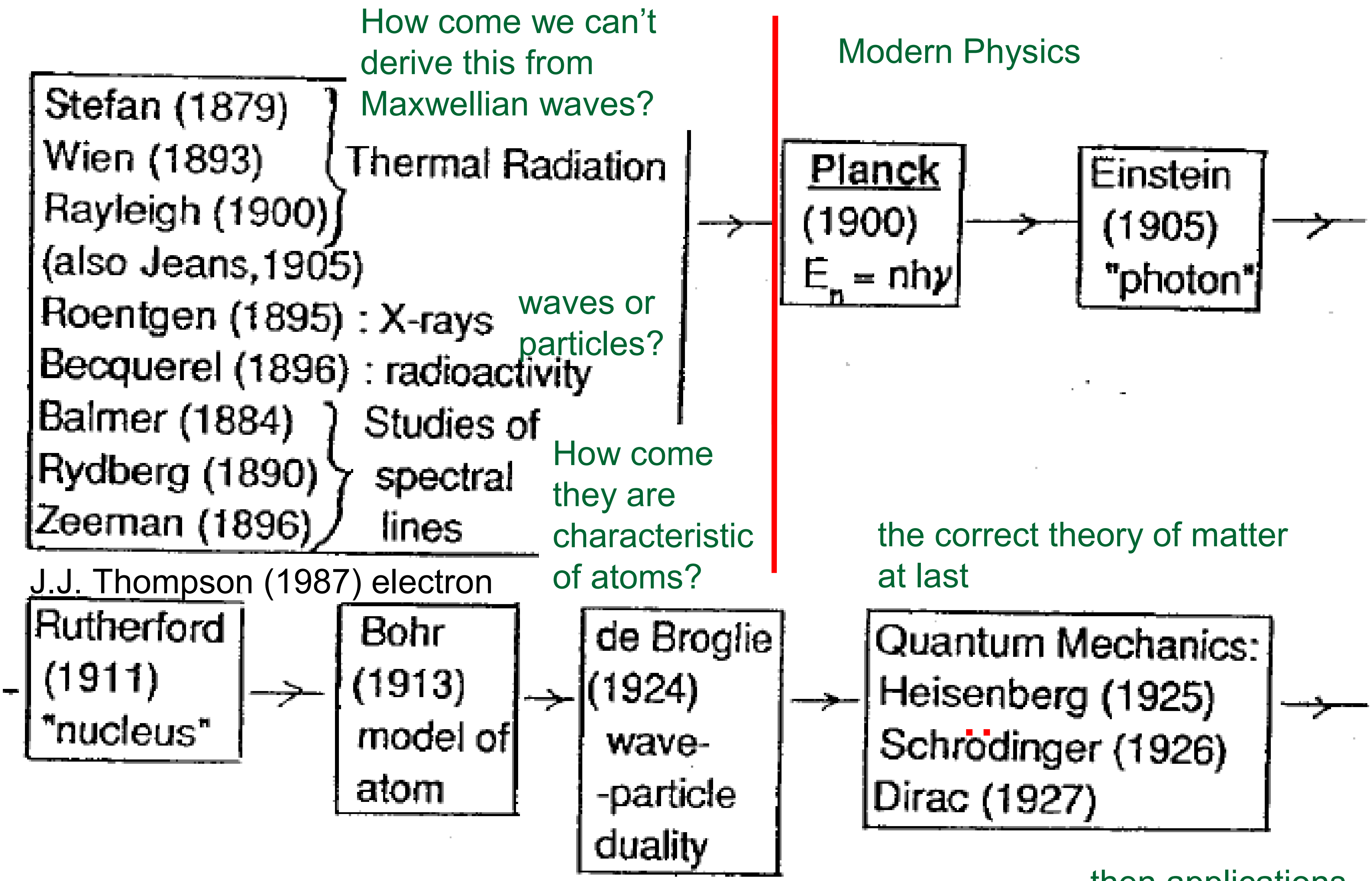
CHAPTER 5

Wave Properties of Matter and Quantum Mechanics I

- 5.1 X-Ray Scattering (review and some more material)
- 5.2 De Broglie Waves
- 5.3 Electron Scattering / Transmission electron microscopy
- 5.4 Wave Motion
- 5.5 Waves or Particles?
- 5.6 Uncertainty Principle
- 5.7 Probability, Wave Functions, double slit experiments, and the Copenhagen Interpretation
- 5.8 Particle in a Box

I thus arrived at the overall concept which guided my studies: for both matter and radiations, light in particular, it is necessary to introduce the corpuscle concept and the wave concept at the same time.

- Louis de Broglie, 1929



How come we can't derive this from Maxwellian waves?

Modern Physics

Stefan (1879)
Wien (1893)
Rayleigh (1900)
(also Jeans,1905)

Thermal Radiation

Roentgen (1895) : X-rays

waves or particles?

Becquerel (1896) : radioactivity

Balmer (1884)
Rydberg (1890)
Zeeman (1896)

Studies of spectral lines

How come they are characteristic of atoms?

Planck
(1900)
$E_n = nh\nu$

Einstein
(1905)
"photon"

the correct theory of matter at last

J.J. Thompson (1987) electron

Rutherford
(1911)
"nucleus"

Bohr
(1913)
model of atom

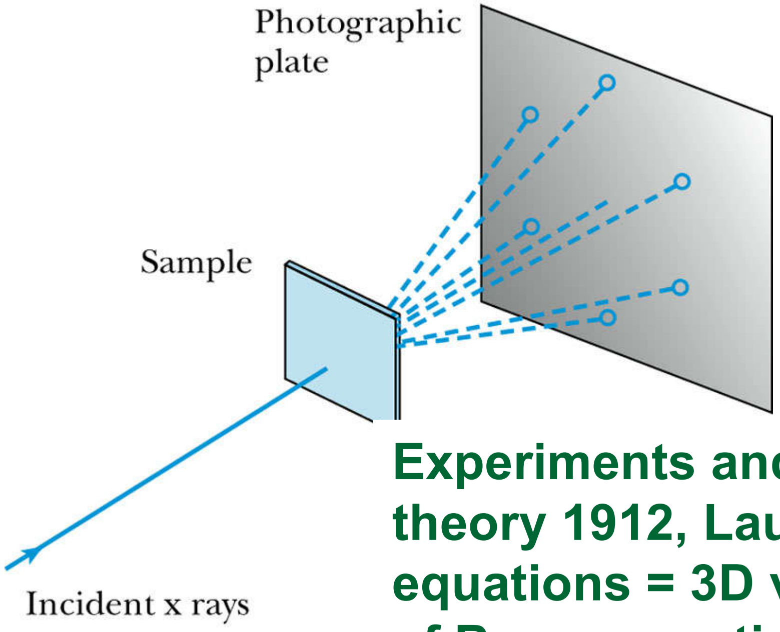
de Broglie
(1924)
wave-
-particle
duality

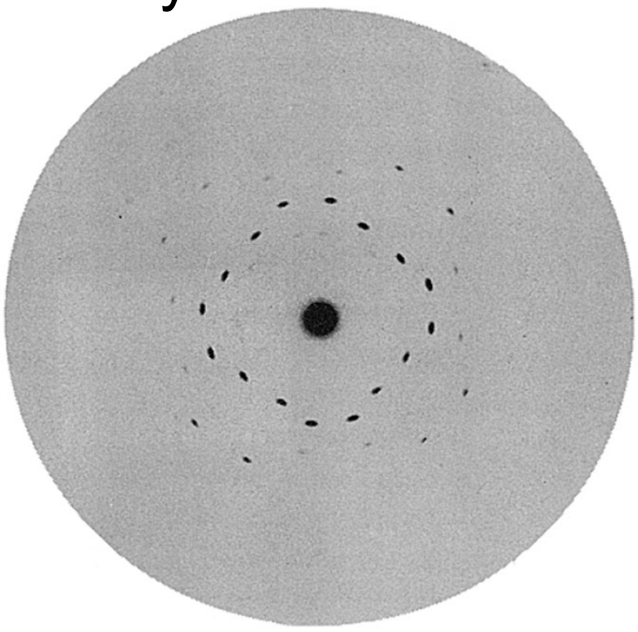
Quantum Mechanics:
Heisenberg (1925)
Schrödinger (1926)
Dirac (1927)

then applications, PH 312

5.1: X-Ray Scattering

- 1912, Max von Laue suggested that if x rays were a form of electromagnetic radiation, interference effects should be observed.
- Crystals act as three-dimensional gratings, scattering the waves and producing observable interference effects shown a few months later experimentally.



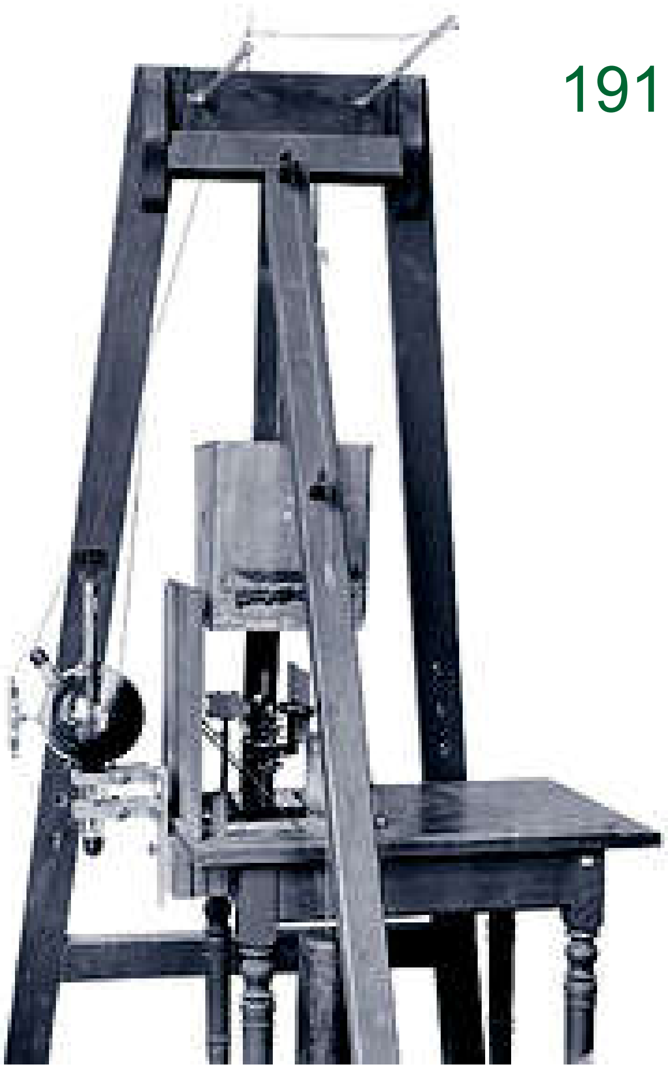


(b)

Experiments and first theory 1912, Laue equations = 3D version of Bragg equation, kinematic theory of X-ray diffraction, Nobel prize 1914

Kinematic theory only single scattering

1912



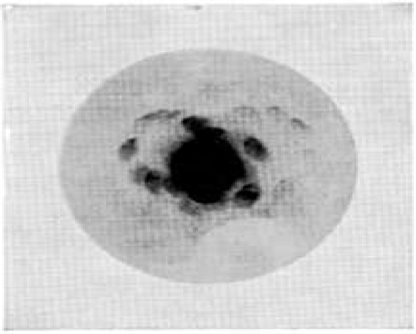


Fig. 4-4(1). Friedrich & Knipping's first successful diffraction photograph.

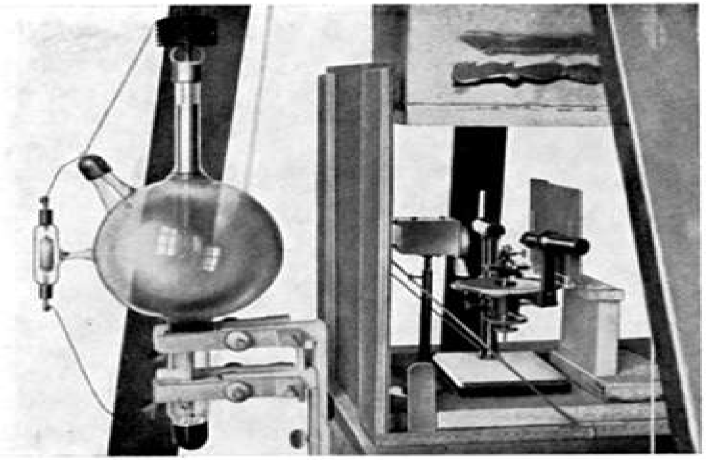
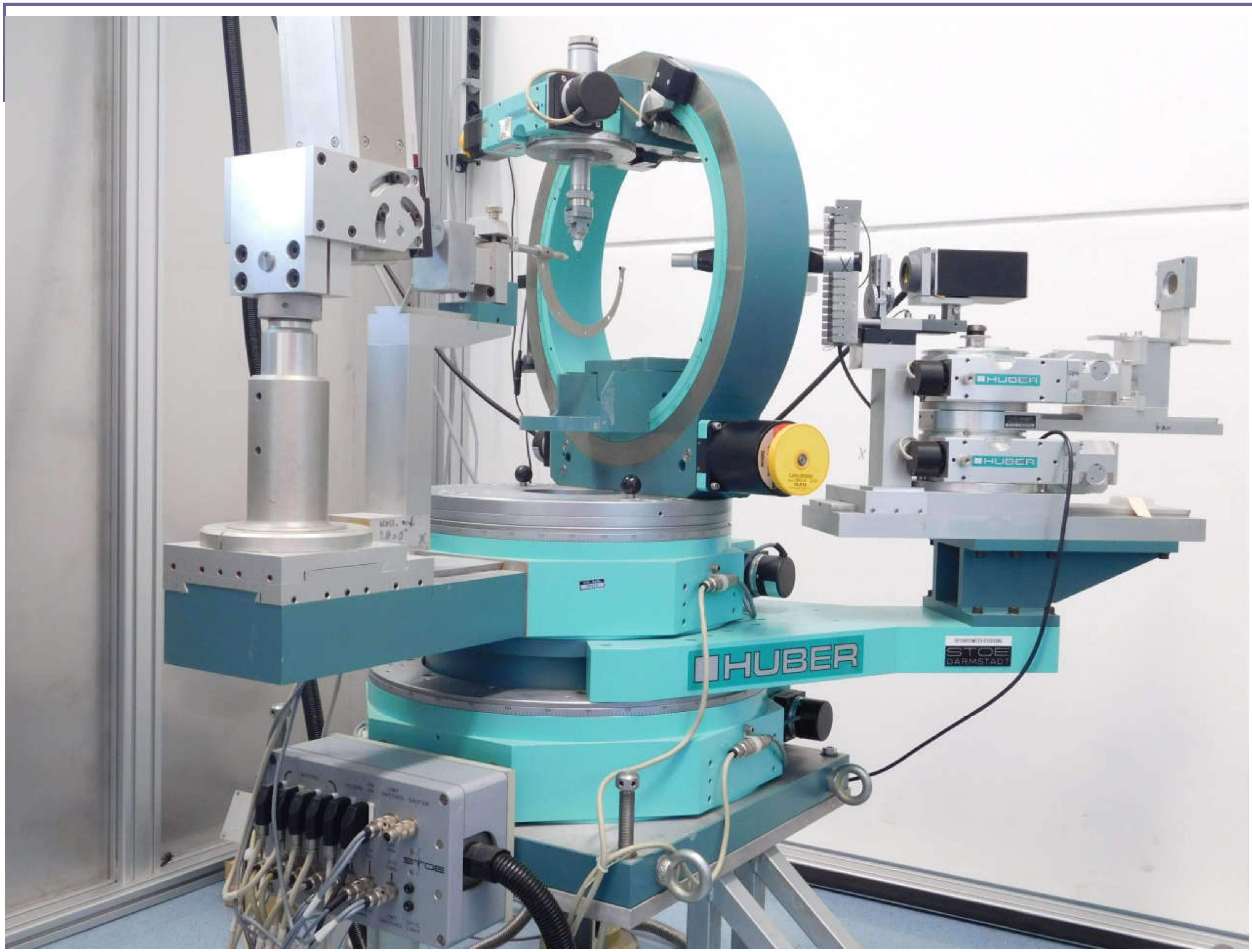
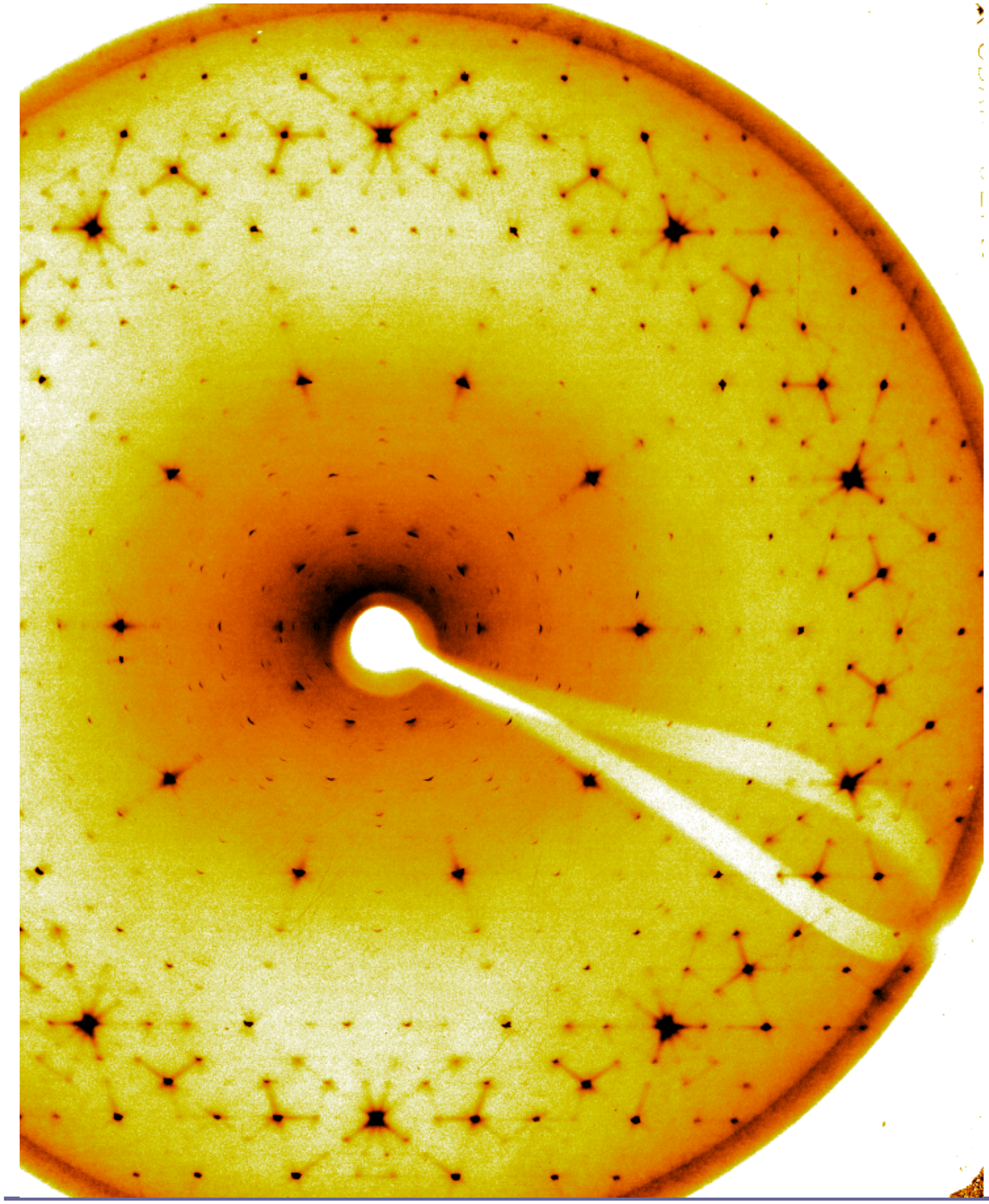


Fig. 4-4(2). Friedrich & Knipping's improved set-up.



Laboratory based single crystal diffractometer



This is actually a quasicrystal, you can tell from the 10 fold rotation symmetry

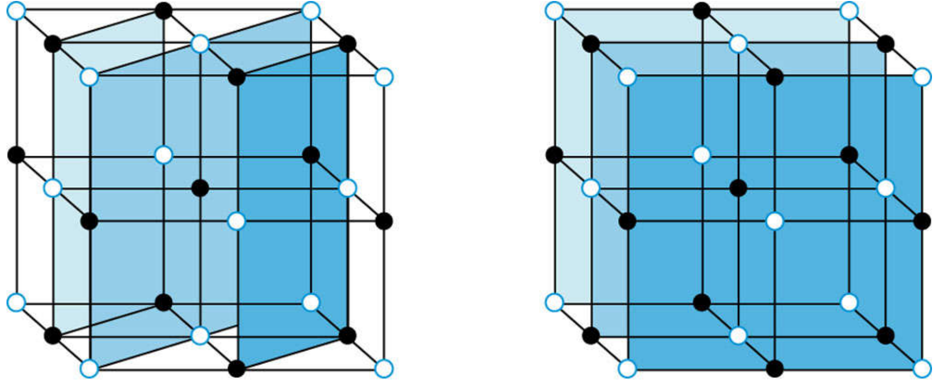
The image is a flat section through reciprocal/Fourier space

As a Fourier transform is a good mathematical model for the diffraction of X-rays by crystals (most ordinary condensed matter) and quasicrystals (some extraordinary condensed matter)

Bragg’s Law revisited

- William Lawrence Bragg (son) interpreted the x-ray scattering as the “specular reflection” (constructive interference) of the incident x-ray beam from a unique set of planes of atoms within the crystal.
- There are two conditions for constructive interference of the scattered x rays:

1) The net plane spacing is so that a path lengths differences arise for the incoming beam that must be an integral number of wavelengths.
2) Angle between incoming and reflected beam must then be 2Θ
3) Only as a byproduct of (1) and (2) the angle of incidence equals the angle of “reflection”



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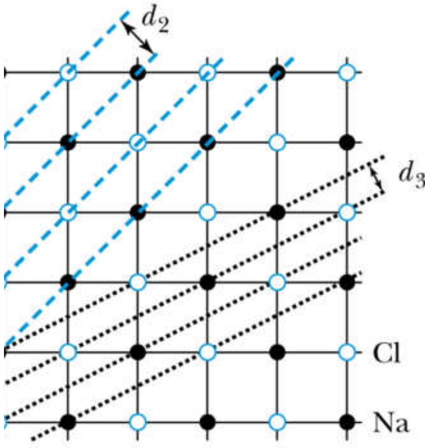

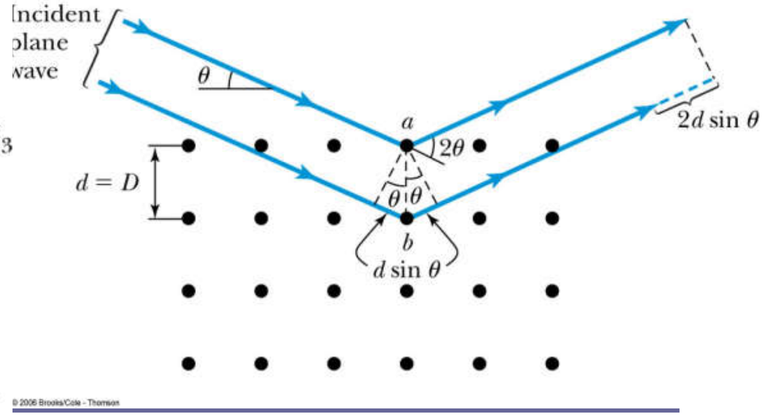

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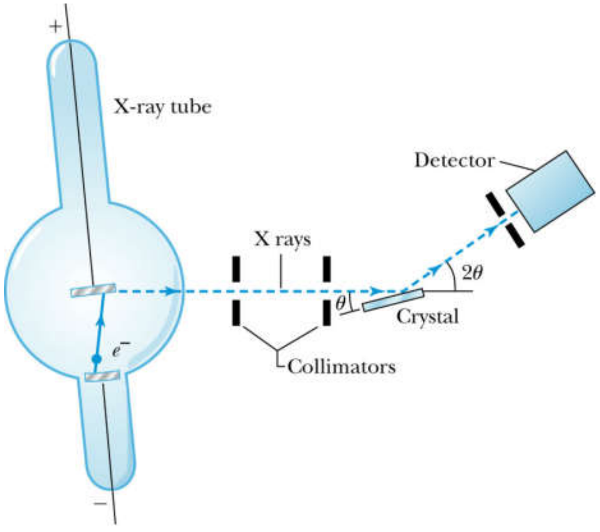
- **Bragg’s Law:**
  $n\lambda = 2d \sin\theta$
  (n = integer)

$$\lambda = 2d_{HKL} \sin\theta$$

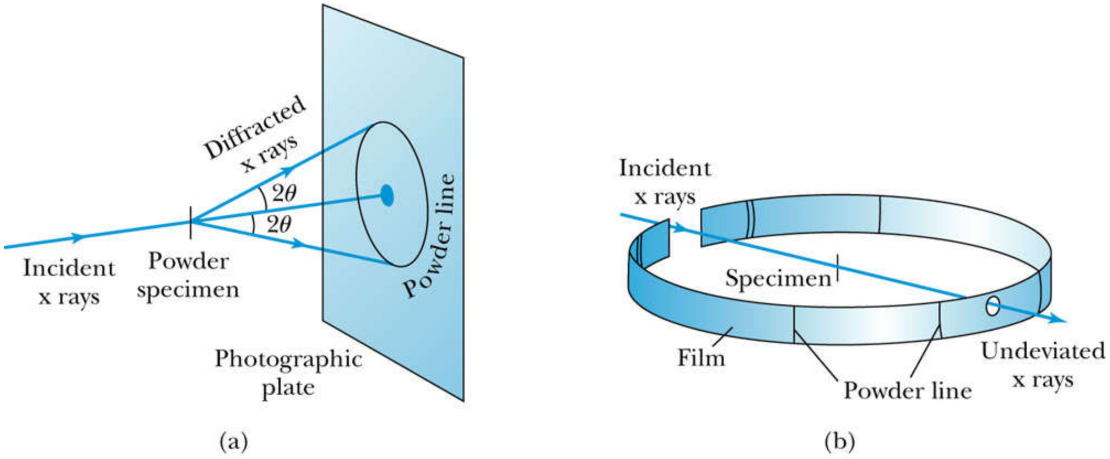
Miller indices hkl, Laue indices HKL

The Bragg Spectrometer

- Bragg spectrometers (invented by Wilhelm Henry Bragg, father) to measure X-ray wavelengths by scattering from crystals. The intensity of a diffracted beam is determined as a function of scattering angle by rotating the crystal and/or the detector. We have seen it used in the Compton experiment

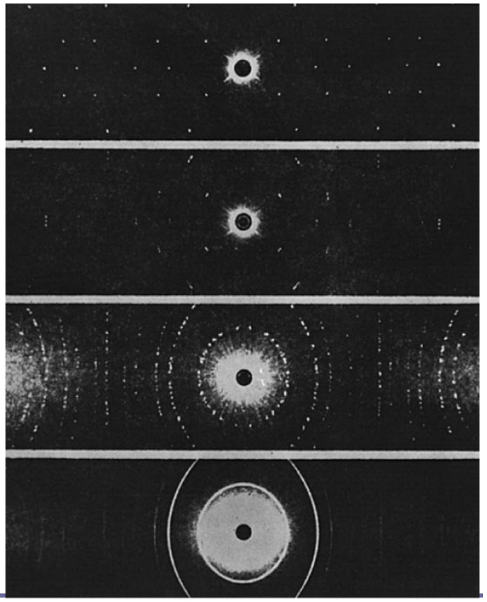


- When a monochromatic beam of X rays passes through the powdered crystal, the dots become a series of rings.



(a)

(b)



(c)

Powder diffractometry is the most important usage of X-rays in industry and possibly for mankind

5.2: De Broglie Waves

- Prince Louis V. de Broglie suggested that massive particles (i.e. matter) should have wave properties similar to electromagnetic radiation.
- The energy can be written analogous to photons $hf = pc = p\lambda f$
- The wavelength of a matter wave is called the de Broglie wavelength (by special relativity there is always a moving observer) so that:

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

I thus arrived at the overall concept which guided my studies: for both matter and radiations, light in particular, it is necessary to introduce the corpuscle concept and the wave concept at the same time.

- Louis de Broglie, 1929

What applies to mass less particles E = pc = hf, i.e. photons, also applies to massive particles – quite strange

We have a second equation for momentum of a massive particle in addition to ***p = mv***

platypus

$$p = h/\lambda = \hbar k$$

for all quantum mechanical particles, not just photons

http://usatoday30.usatoday.com/tech/science/genetics/2008-05-08-platypus-genetic-map_N.htm, *Ornithorhynchus anatinus, platipus*

“Australia's unique duck-billed platypus is part bird, part reptile and part mammal according to its gene map.

The platypus is classed as a mammal because it has fur and feeds its young with milk. They hatch from eggs. It flaps a beaver-like tail. But it also has bird and reptile features — a duck-like bill and webbed feet, and lives mostly underwater. Males have venom-filled spurs on their heels.”

Bohr's Quantization Condition / standing waves

- Bohr's crucial assumptions concerning his hydrogen atom model was that the angular momentum of the electron-nucleus system in a stationary state is an integral multiple of *h*/2*π*.
- One can justify this by saying that the electron is a standing wave (in an circular orbit) around the proton. This standing wave will have nodes and be an integral number of wavelengths.

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

$$2\pi r = n\lambda = n\frac{h}{p}$$

- The angular momentum becomes:

$$L = rp = \frac{nh}{2\pi} = n\hbar$$

Which is identical to Bohr's crucial assumption

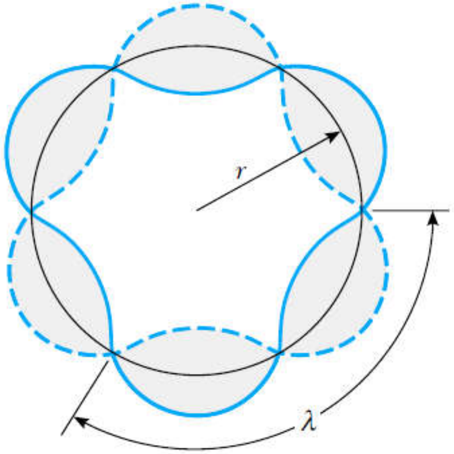
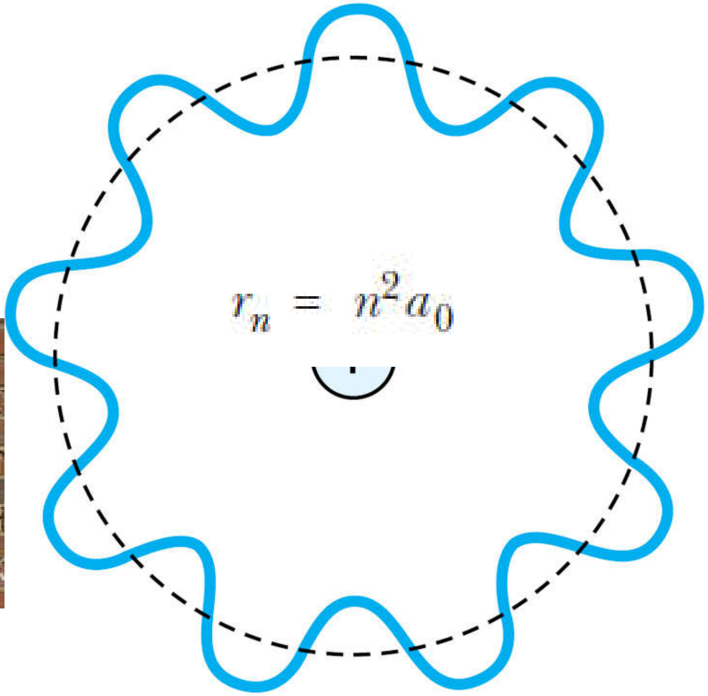


Figure 5.2 Standing waves fit to a circular Bohr orbit. In this particular diagram, three wavelengths are fit to the orbit, corresponding to the $n = 3$ energy state of the Bohr theory.

Linear momentum is quantized as well, how come ? because total energy is quantized in bound systems !!

The important new physics is that the electron is some kind of a standing wave that reinforces itself while orbiting the proton, circumference circle 2π r

If the wave is along the circumference of a circle, that works, but there are many other possible scenarios



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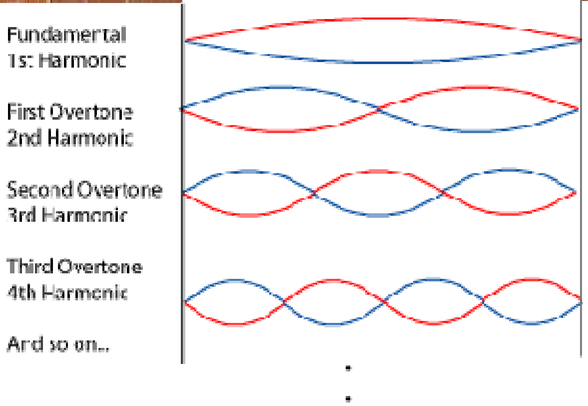
$$1^2 = w_1$$

$$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{me^2} 2\pi$$



$2^2\, w_2$

$3^2\, w_3$

$4^2\, w_4$

for all higher harmonics, 2, 3, …walls need to be apart distances $w_n = n^2\, 2\pi\, a_0$

While this model is aesthetically less pleasing, it gives the very same predictions as the Bohr model, so is for physics just as good, linear momentum is quantized here

So a “charged wave-particle thingy in a set of boxes model” makes the same predictions, we only need to fix the widths of the boxes to certain values of a certain constant and quantum jumps are then from one box to the next.

The features of this model are that De Broglie’s equation is valid, we have standing waves, and integral number of waves need to fit into the box in order to make them a standing wave, with that we have linear momentum and kinetic energy quantized, no need to consider any potential energy, so total energy is quantized – isn’t that great and ridiculous

Since this model is in agreement with experimental evidence, it has just as much predictive power as the Bohr model (but disagrees with Rutherford’s experiment)

can claim to be just as right (or just as ridiculous) as the Bohr model - for the purpose of explaining spectral lines - with the electron (particle) going around the positively charged nucleus (another particle) in a circle

Bound system, particle in a box, it persist to exist, does not blow up, does not disappear by some miraculous process, is always there going back and forth between the walls, won’t stand still

5.3: Electron Scattering/Diffraction

Any experimental evidence?
sure in abundance

Several
tens of V,
so low
energy
eV

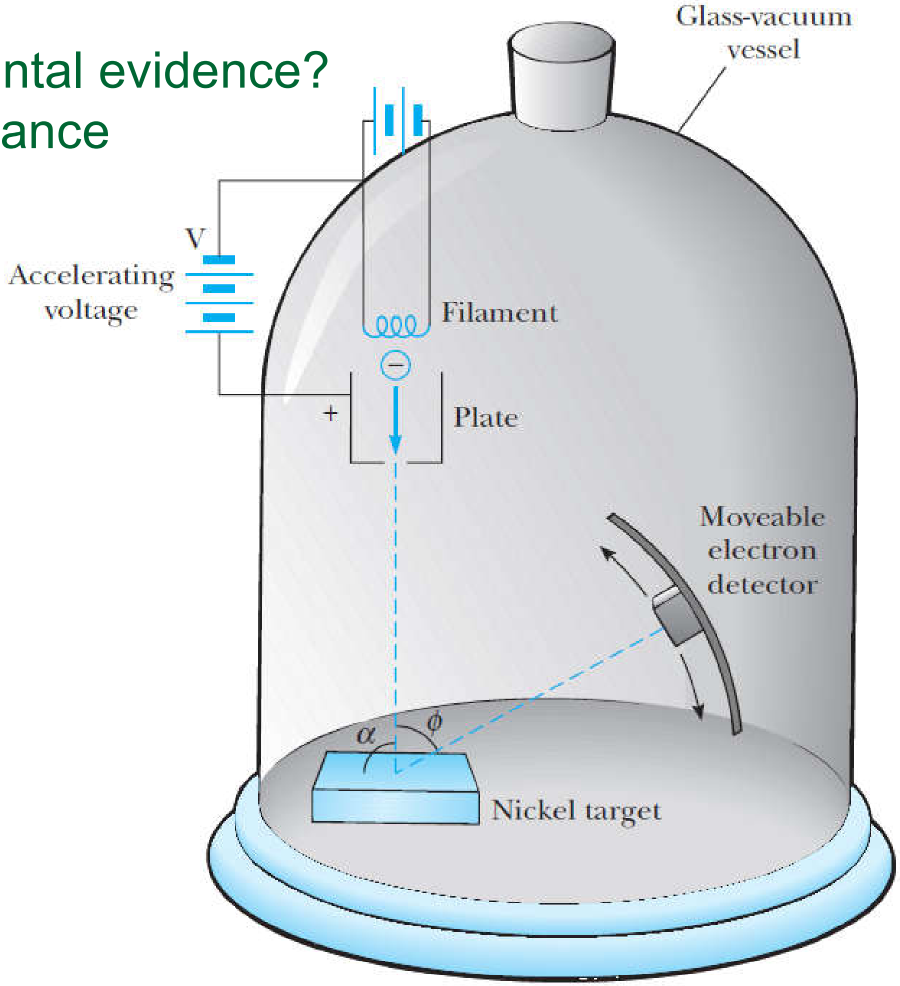


Figure 5.4 A schematic diagram of the Davisson–Germer apparatus.

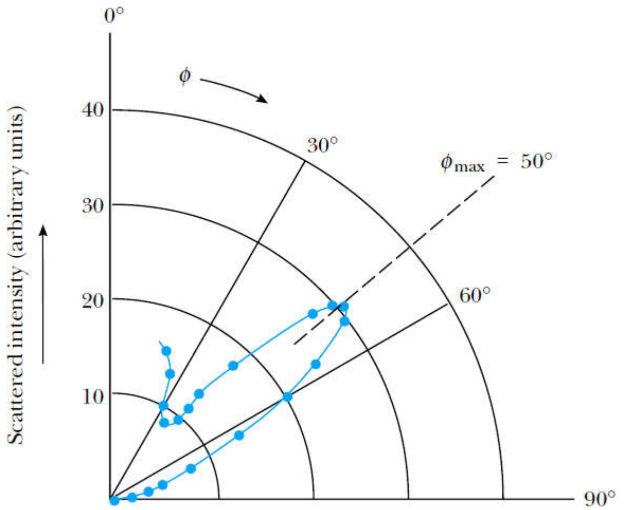


Figure 5.5 A polar plot of scattered intensity versus scattering angle for 54-eV electrons, based on the original work of Davisson and Germer. The scattered intensity is proportional to the distance of the point from the origin in this plot.

Figure 5-4 Scattering of electrons by a crystal. Electron waves are strongly scattered if the Bragg condition $n\lambda = 2d \sin\theta$ is met. This is equivalent to the condition $n\lambda = D \sin\varphi$.

Between incident beam and reflected beam, there is always 2Θ, the glancing angle, with Θ as Bragg angle

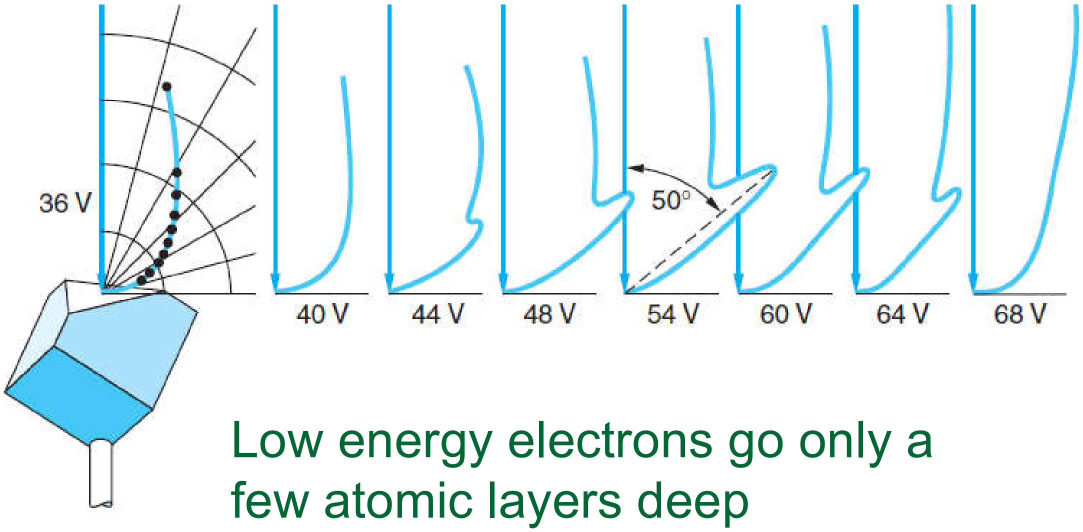


Figure 5-6 A series of polar graphs of Davisson and Germer's data at electron accelerating potentials from 36 V to 68 V. Note the development of the peak at $\varphi = 50°$ to a maximum when $V_0 = 54$ V.

Low energy electrons go only a few atomic layers deep

$$\alpha = 90.0^\circ,\ V = 54.0\ \text{V, and}\ \phi = 50.0^\circ$$

$$\tfrac{1}{2} m_e v^2 = eV \qquad v = \sqrt{2Ve/m_e}$$

$$\lambda = \frac{h}{m_e v} = \frac{h}{\sqrt{2Vem_e}}$$

$$\lambda = \frac{6.63 \times 10^{-34}\ \text{J}\cdot\text{s}}{\sqrt{2(54.0\ \text{V})(1.60 \times 10^{-19}\ \text{C})(9.11 \times 10^{-31}\ \text{kg})}}$$
$$= 1.67 \times 10^{-10}\ \text{m} = 1.67\ \text{Å}$$

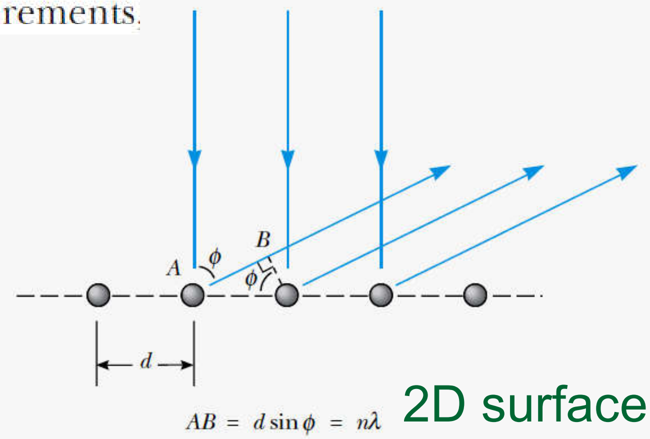
As the energy of the electrons is so low, resulting in speeds much below 1% of c, we can use classical physics for momentum for these particles with mass, (many GeV to TeV in accelerators are relativistic particles)

d was known to be 2.15 Å from x-ray diffraction measurements.

$$d \sin \phi = n\lambda$$

$$\lambda = (2.15\ \text{Å})(\sin 50.0^\circ) = 1.65\ \text{Å}$$

Note that this d is not a net plane spacing, it's one of the shortest distances of the 2D surface arrangement of atoms

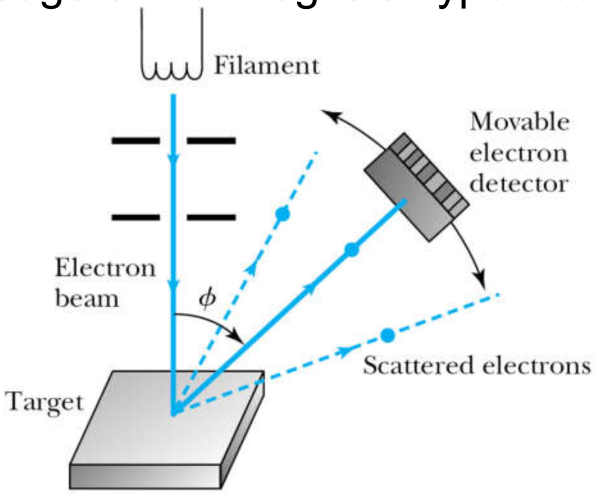


2D surface grating

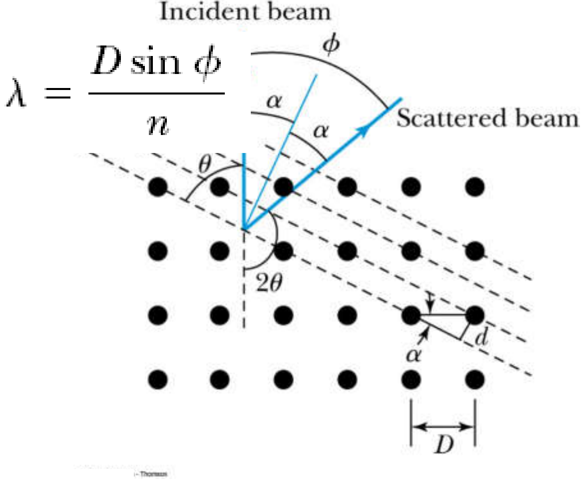
Figure 5.6 Constructive interference of electron matter waves scattered from a single layer of atoms at an angle ϕ.

Rows of atoms act as surface grating, note that this is not W. L. Bragg's diffraction equations, but the same kind of effect

- **Davisson** and Germer experimentally observed that electrons were diffracted much like x rays in nickel crystals, just trying to continue with prior research, no knowledge of De Broglie’s hypothesis at that time

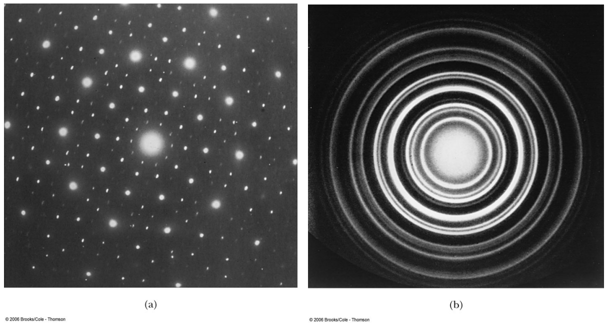


$\sin \gamma = \sin (180 - \gamma)$

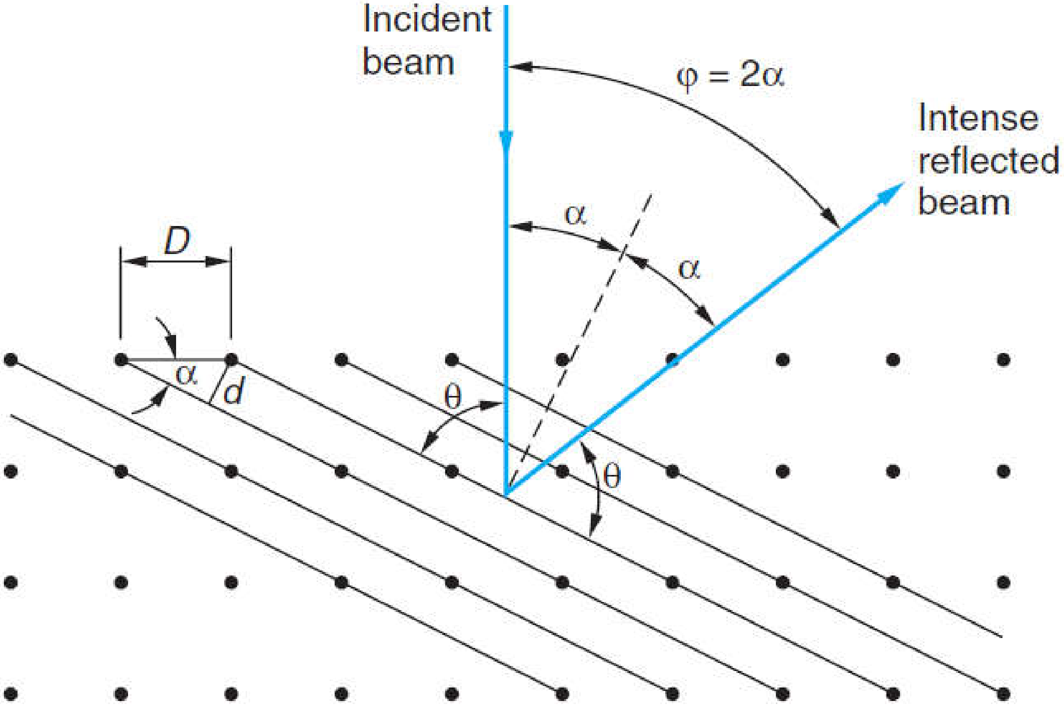


$D = {}^{d}/_{\sin \alpha}$

- **George P. Thomson** (1892–1975), son of J. J. Thomson, knew about De Broglie’s hypothesis and set out to prove (or disprove) it, build the first high energy electron diffraction camera
- reported seeing the effects of electron diffraction in transmission experiments. The first target was celluloid, and soon after that gold, aluminum, and platinum were used. The randomly oriented polycrystalline sample of SnO_2 produces rings as shown in the figure at right.


(a) (b)

Nobel prize 1937



$$\lambda = 2d_{HKL} \sin \Theta$$

Bragg equation

$$D = {}^{d}/_{\sin \alpha}$$

$$2\varphi = 4\alpha = 2\,(90^{o} - \Theta)$$

$$\sin 2\varphi = \sin 180^{o} - 2\Theta$$

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE_k}}$$

When acceleration voltages are small, we can get away with the non-relativistic expression for KE, E_K

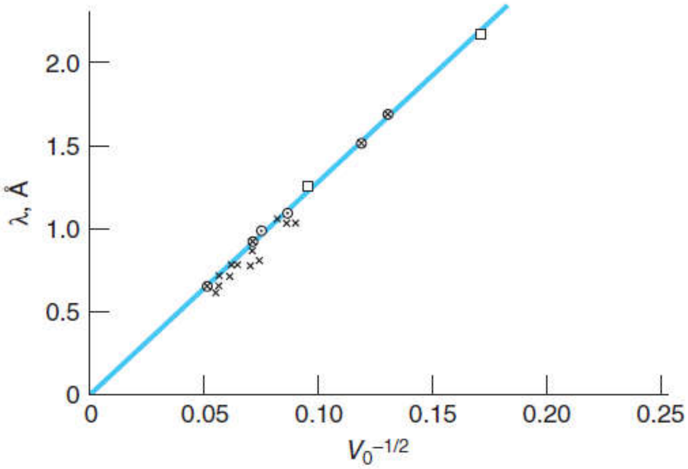
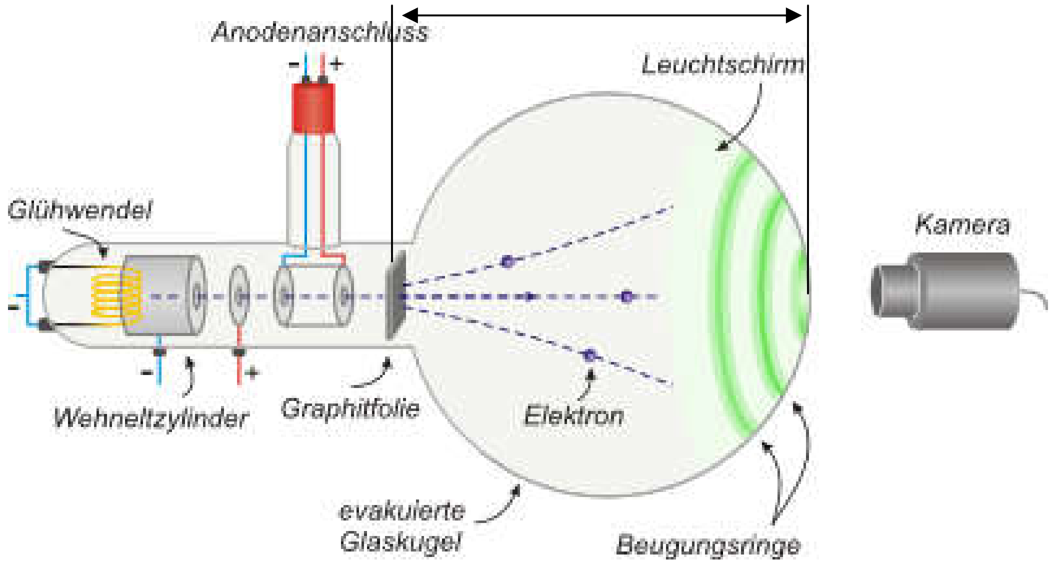


Figure 5-5 Test of the de Broglie formula $\lambda = h/p$. The wavelength is computed from a plot of the diffraction data plotted against $V_0^{-1/2}$, where V_0 is the accelerating voltage. The straight line is $1.226V_0^{-1/2}$ nm as predicted from $\lambda = h(2mE)^{-1/2}$. These are the data referred to in the quotation from Davisson's Nobel lecture. (× From observations with diffraction apparatus; ⊗ same, particularly reliable; □ same, grazing beams. ⊙ From observations with reflection apparatus.) [*From Nobel Prize Lectures: Physics (Amsterdam and New York: Elsevier, © Nobel Foundation, 1964).*]

Here is Davisson's account of the connection between de Broglie's predictions and their experimental verification:

> Perhaps no idea in physics has received so rapid or so intensive development as this one. De Broglie himself was in the van of this development, but the chief contributions were made by the older and more experienced Schrödinger. It would be pleasant to tell you that no sooner had Elsasser's suggestion appeared than the experiments were begun in New York which resulted in a demonstration of electron diffraction—pleasanter still to say that the work was begun the day after copies of de Broglie's thesis reached America. The true story contains less of perspicacity and more of chance. . . It was discovered, purely by accident, that the intensity of elastic scattering [of electrons] varies with the orientations of the scattering crystals. Out of this grew, quite naturally, an investigation of elastic scattering by a single crystal of predetermined orientation. . . Thus the New York experiment was not, at its inception, a test of wave theory. Only in the summer of 1926, after I had discussed the investigation in England with Richardson, Born, Franck and others, did it take on this character.[7]

the technique is now known as low energy electron diffraction (LEED) and a valuable surface characterization tool that needs ultra high vacuum for clean surfaces camera lengths, l



$p = m_e \cdot v$ particle

$m_e \cdot v = \hbar \cdot k$ wave $\Leftrightarrow m_e \cdot v = \frac{h}{\lambda} \quad \Leftrightarrow \lambda = \frac{h}{m_e \cdot v}.$

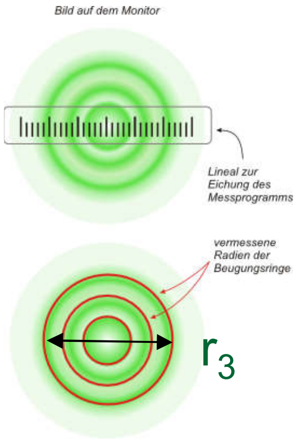
$\frac{1}{2} m_e \cdot v^2 = e \cdot U$ energy balance $\Leftrightarrow v = \sqrt{\frac{2e \cdot U}{m_e}}. \quad \lambda = \frac{h}{\sqrt{2 m_e e U}}.$

$2d \sin \alpha_n = n \cdot \lambda$

Bragg equation, typically Θ, between primary beam and diffracted beams always 2 Θ

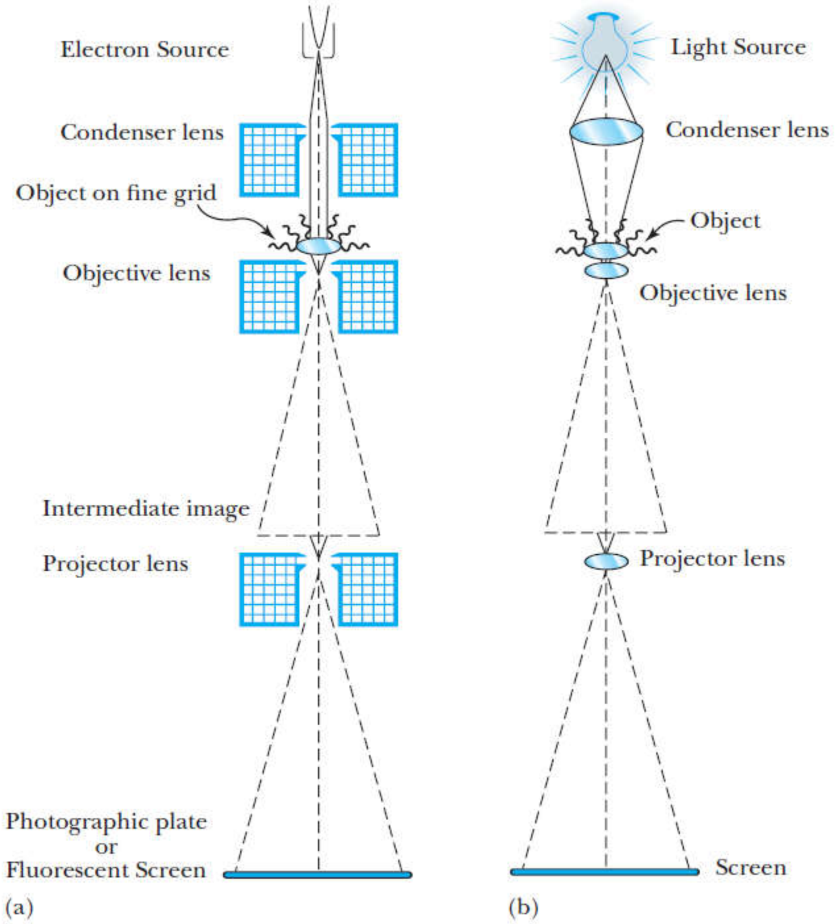
either l >> r_n
or flat screen
(both in TEM)

$$\tan 2\alpha_n = \frac{r_n}{l}.$$



By measuring r_n and knowing l *one can determine the ratio λ/d, characteristic of the crystalline material !!! But why are there rings??*

TEM



(a) (b)

Figure 5.11 (a) Schematic drawing of a transmission electron microscope with magnetic lenses. (b) Schematic of a light-projection microscope.

- Typical acceleration voltages are hundreds of thousands of eV

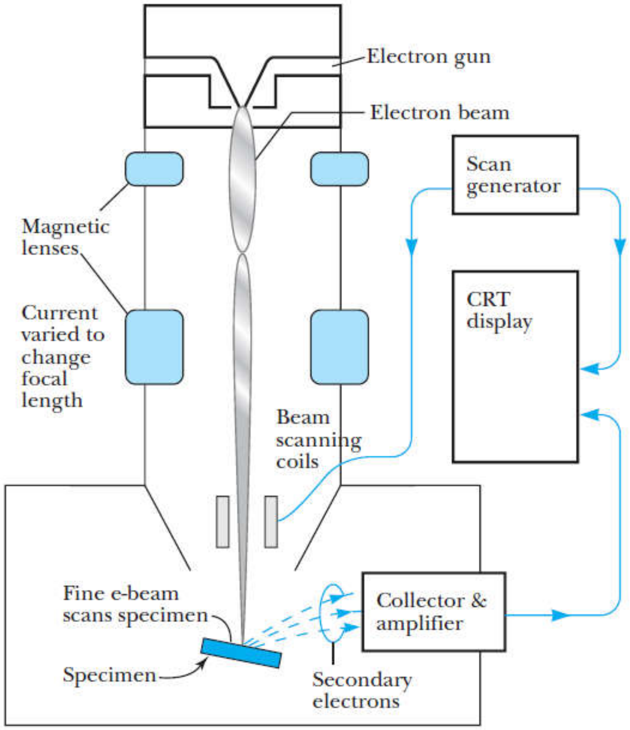


Figure 5.15 The working parts of a scanning electron microscope.

SEM

Typical acceleration voltages are tens of thousands of eV

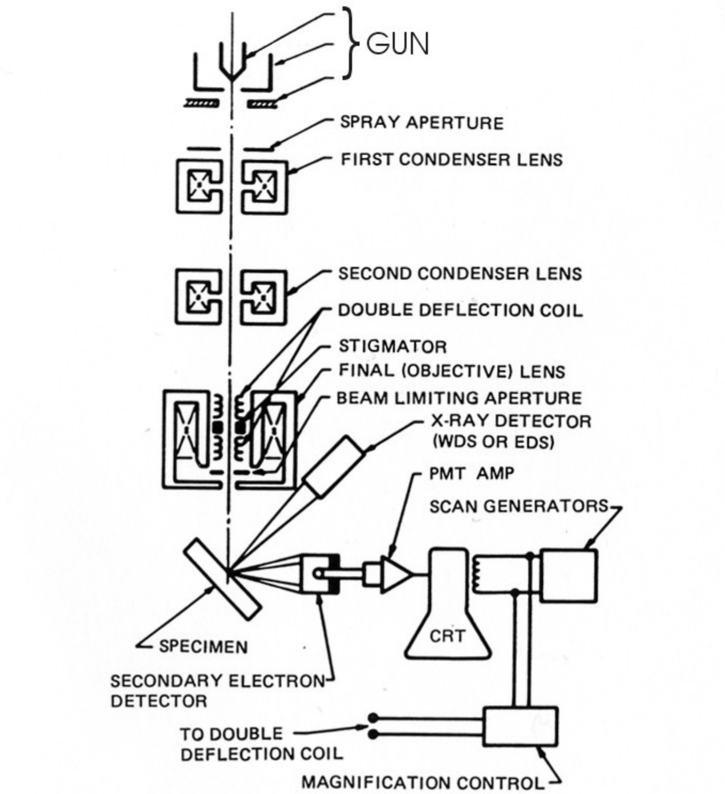
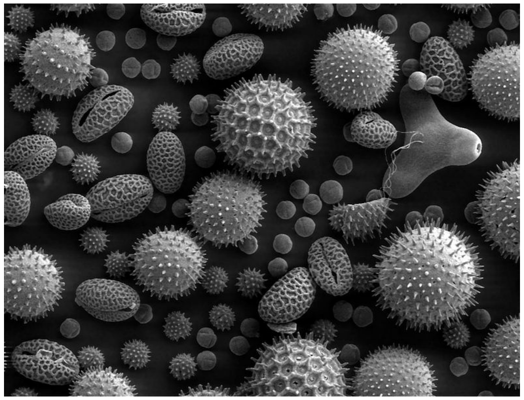
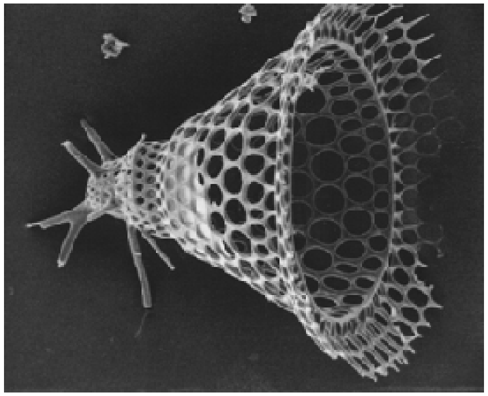


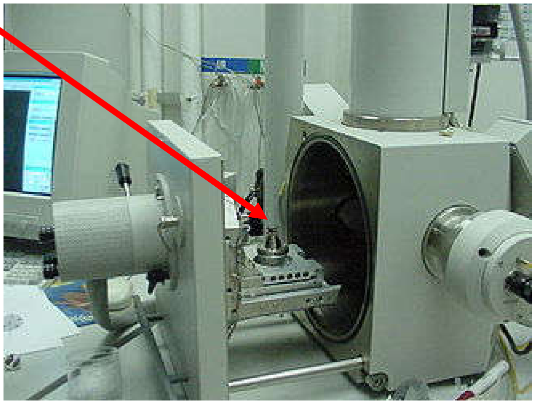
Figure 1.11. Schematic drawing of the electron and x-ray optics of a combined SEM–EPMA.

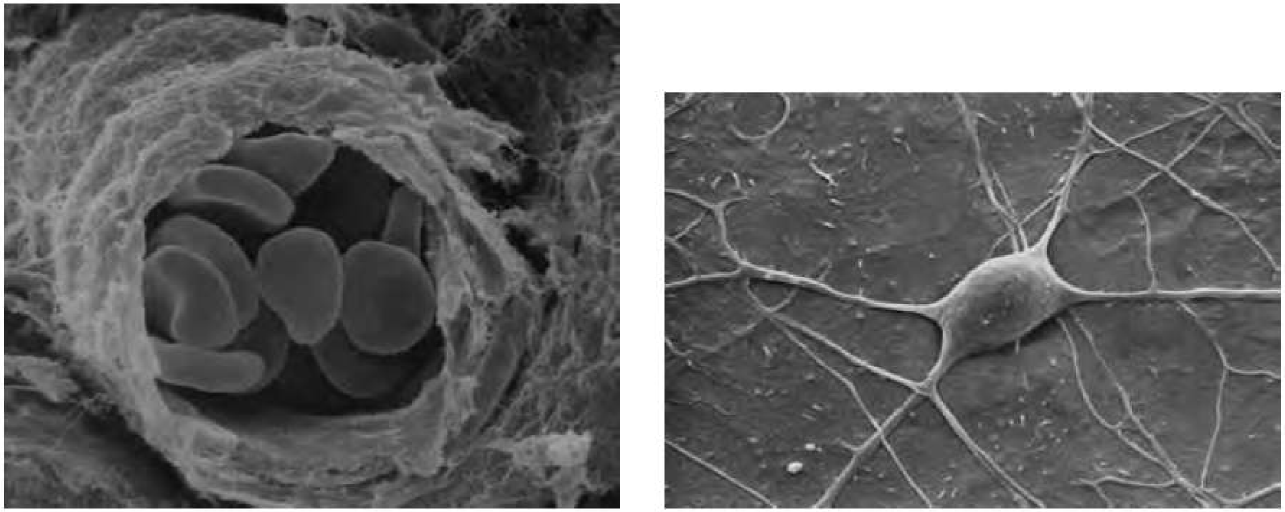




Is there something very important missing in these images ???

dead spider with a thin coating of Au in order to make it conductive for better image contrast

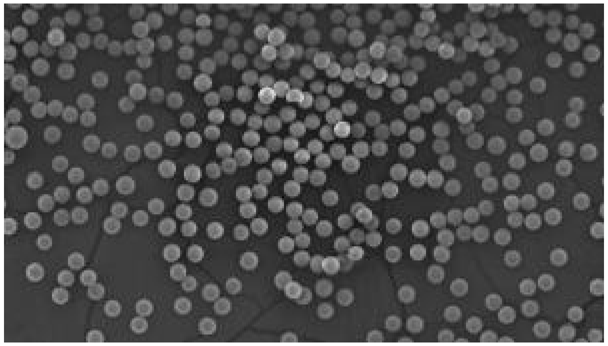




(a) (b)

Figure 5.14 (a) A SEM micrograph showing blood cells in a tiny artery. (b) A SEM micrograph of a single neuron (×4000). (*P. Motta & S. Correr/Photo Researchers, Inc., David McCarthy/Photo Researchers, Inc.*)

Alternatively, one may give the magnification, but it is “bad taste” in the community of electron microscopists http://en.wikipedia.org/wiki/File:SEM_Zoom.ogg

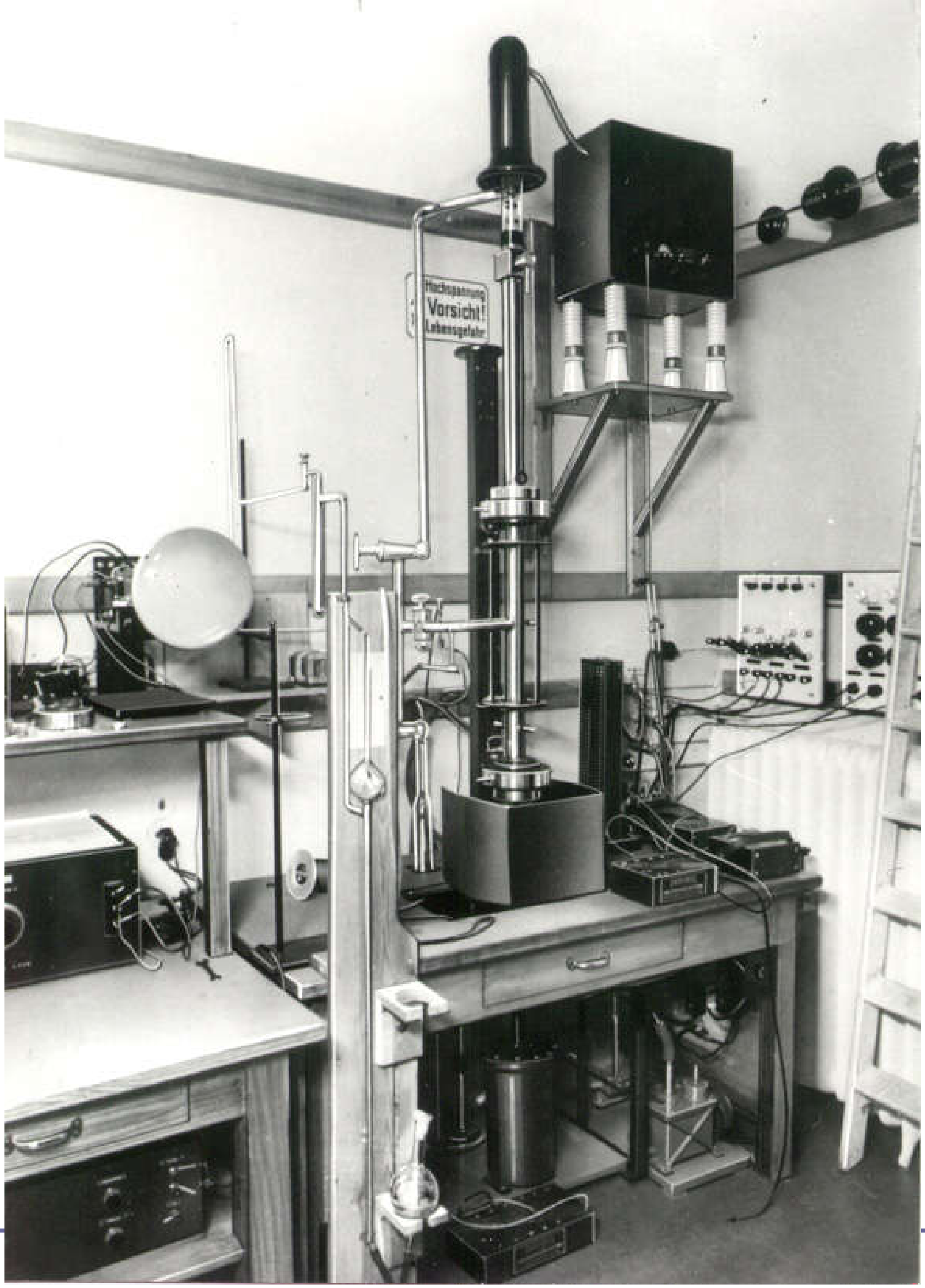


The video starts at 25x, about 6 mm across the whole field of view, and zooms in to 12000x, about 12 μm across the whole field of view. The spherical objects are glass beads with a diameter of 10 μm, similar in diameter to a red blood cell.

Magnification of a couple of hundred thousand times are possible with modern SEMs world’s first ever SEM (with transmission capabilities, so also a STEM)

Count Manfred von Ardenne, (the red baron), 1937

No academic affiliation, private laboratory, partly sponsored by the German post office as part of the development of television



Commercialized as late as 1965 in England, later on in Germany and many other manufactures including FEI

Table top SEM, 350,000 x, 15 keV, with inbuilt spectrometer for characteristics X-rays

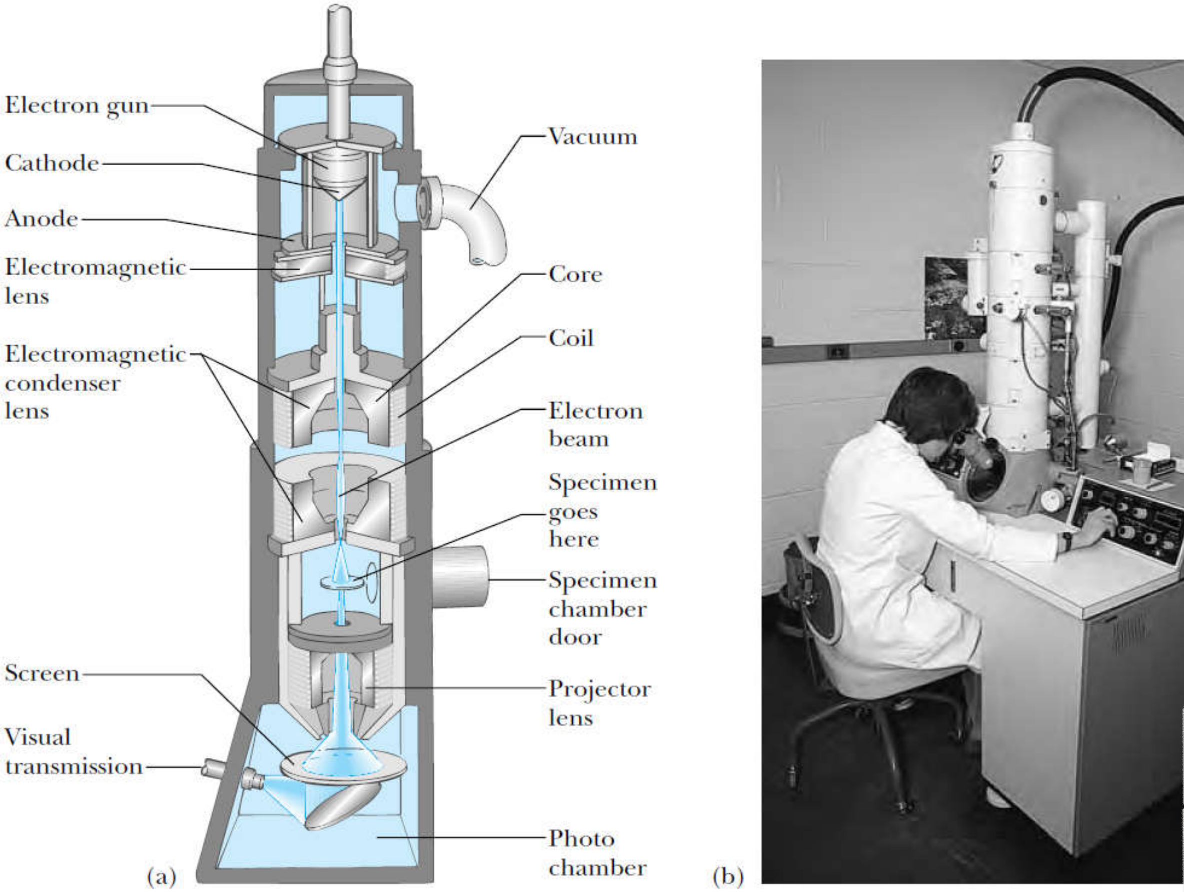
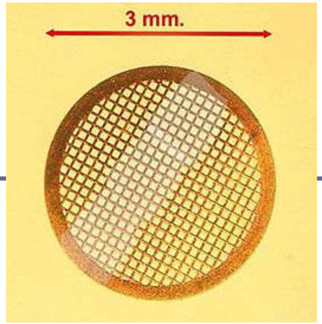
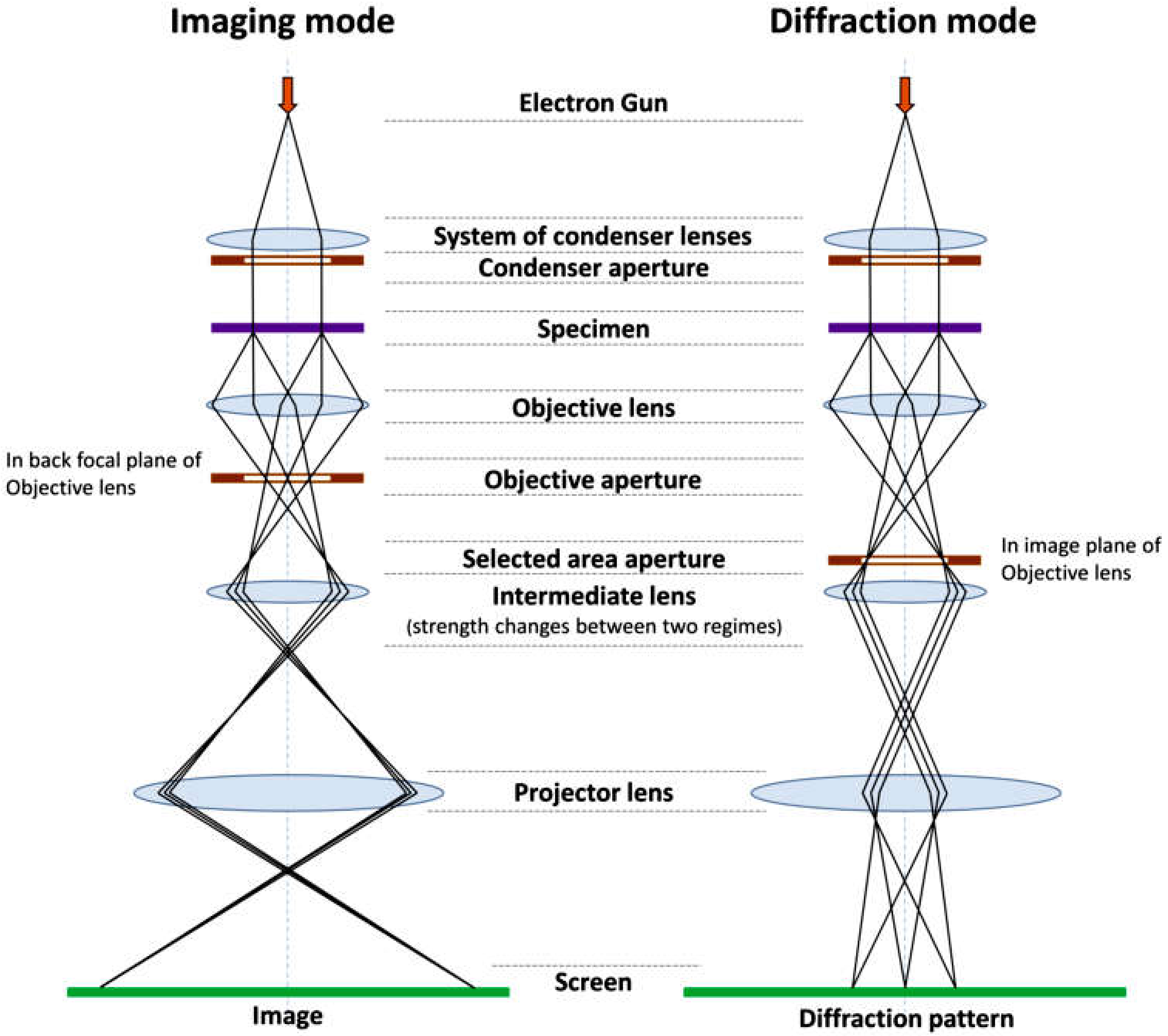


Figure 5.13 (a) Diagram of a transmission electron microscope. (b) A p
same TEM. (*W. Ormerod/ Visuals Unlimited*)

Tomography: http://en.wikipedia.org/wiki/Transmission_electron_microscopy





Imaging mode

Diffraction mode

Electron Gun

System of condenser lenses

Condenser aperture

Specimen

Objective lens

In back focal plane of
Objective lens

Objective aperture

Selected area aperture

In image plane of
Objective lens

Intermediate lens
(strength changes between two regimes)

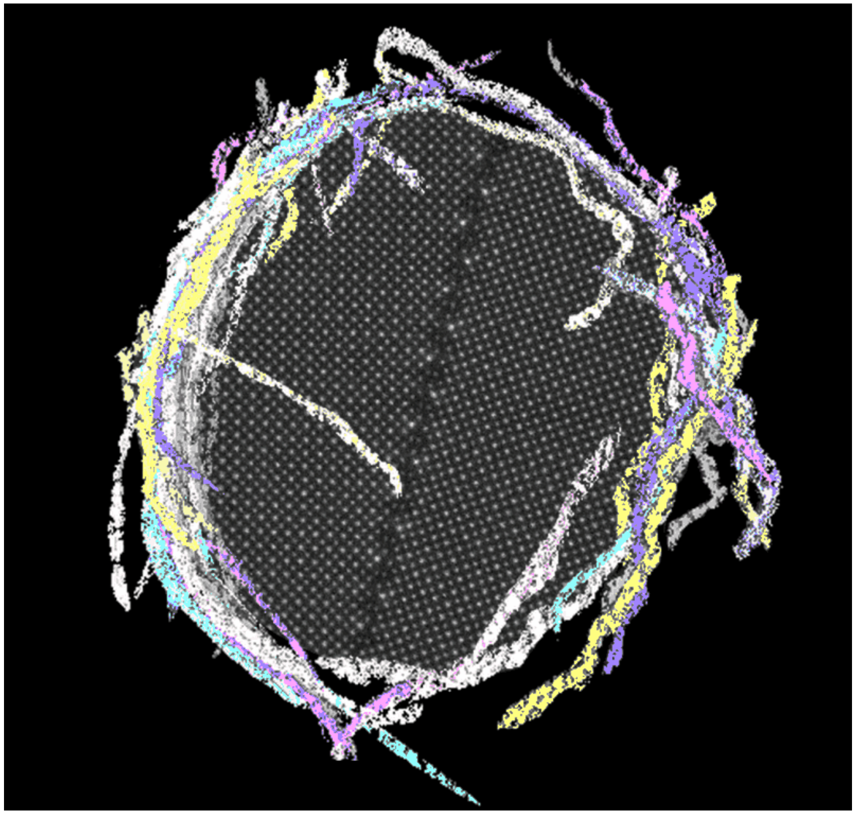
Projector lens

Screen

Image

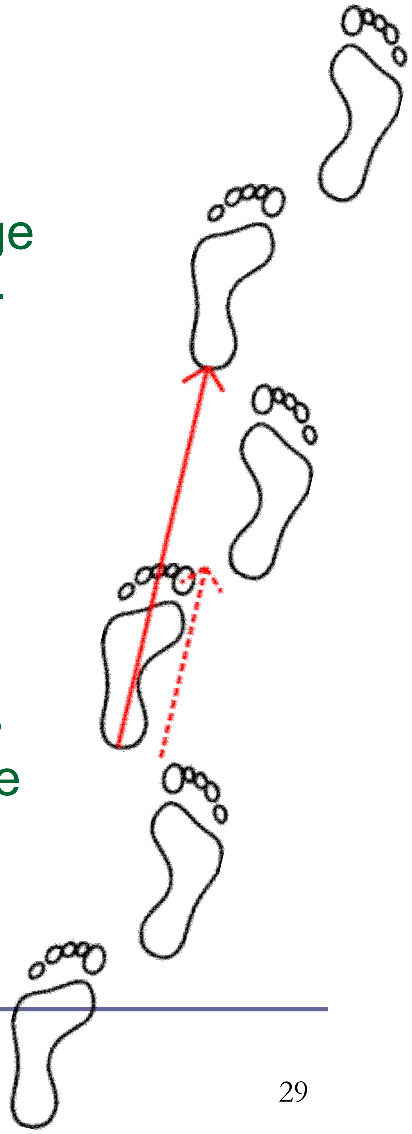
Diffraction pattern

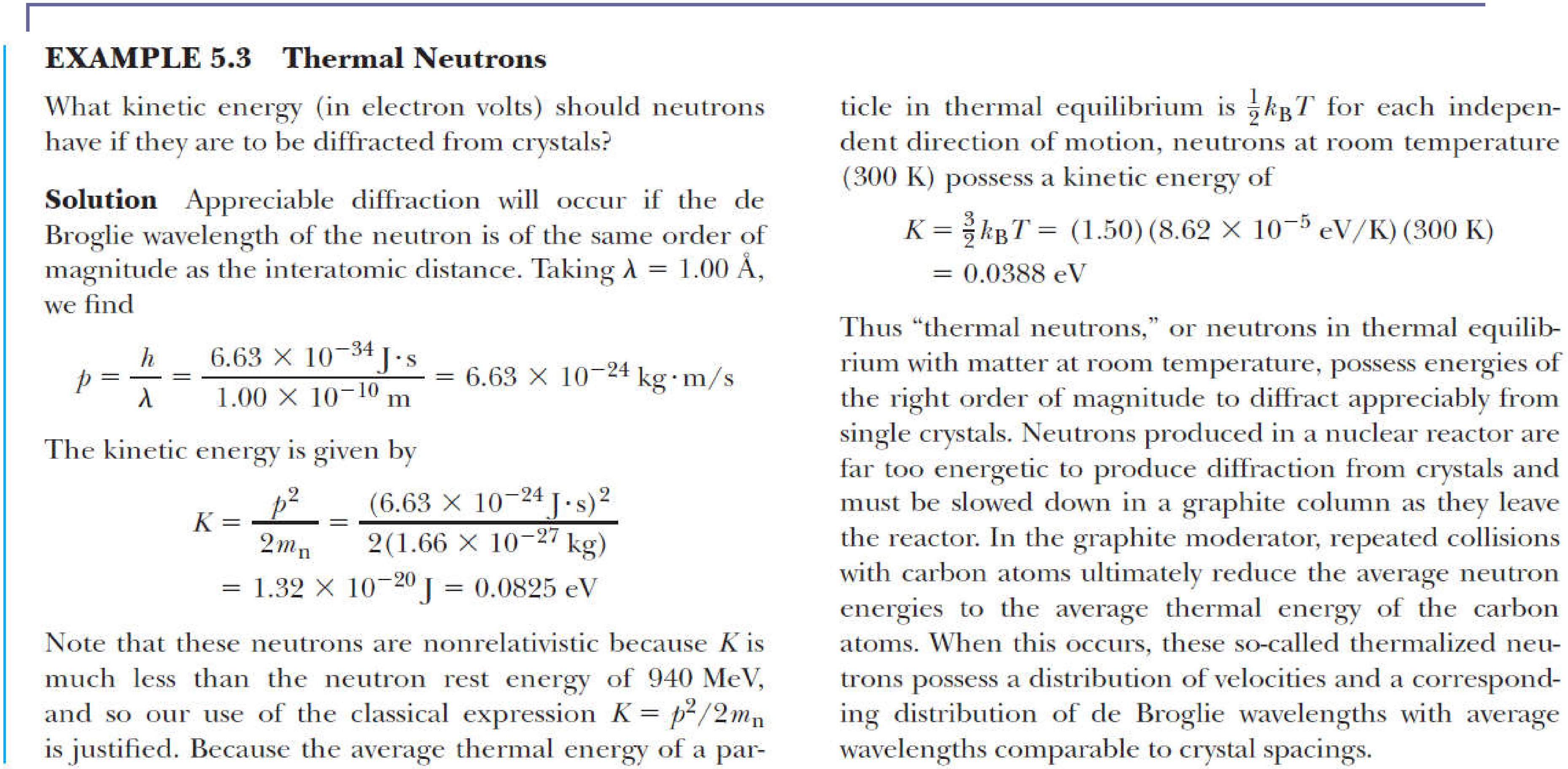
Logo of the Springer-Nature on-line journal "Advanced Structural and Chemical Imaging"



combines an atomic resolution Z-contrast image of a grain boundary in Eu-doped $SrTiO_3$ with an *in situ* image of FtsZ type filaments (proteins) of *Arabidopsis thaliana* wrapped around.

the spacing of Sr atoms is approximately 0.4 nm. The frieze group of the grain boundary is *p11g*





EXAMPLE 5.3 Thermal Neutrons

What kinetic energy (in electron volts) should neutrons have if they are to be diffracted from crystals?

Solution Appreciable diffraction will occur if the de Broglie wavelength of the neutron is of the same order of magnitude as the interatomic distance. Taking $\lambda = 1.00$ Å, we find

$$p = \frac{h}{\lambda} = \frac{6.63 \times 10^{-34}\,\mathrm{J\cdot s}}{1.00 \times 10^{-10}\,\mathrm{m}} = 6.63 \times 10^{-24}\,\mathrm{kg\cdot m/s}$$

The kinetic energy is given by

$$K = \frac{p^2}{2m_\mathrm{n}} = \frac{(6.63 \times 10^{-24}\,\mathrm{J\cdot s})^2}{2(1.66 \times 10^{-27}\,\mathrm{kg})}$$
$$= 1.32 \times 10^{-20}\,\mathrm{J} = 0.0825\ \mathrm{eV}$$

Note that these neutrons are nonrelativistic because K is much less than the neutron rest energy of 940 MeV, and so our use of the classical expression $K = p^2/2m_\mathrm{n}$ is justified. Because the average thermal energy of a particle in thermal equilibrium is $\frac{1}{2}k_\mathrm{B}T$ for each independent direction of motion, neutrons at room temperature (300 K) possess a kinetic energy of

$$K = \tfrac{3}{2}k_\mathrm{B}T = (1.50)(8.62 \times 10^{-5}\ \mathrm{eV/K})(300\ \mathrm{K})$$
$$= 0.0388\ \mathrm{eV}$$

Thus "thermal neutrons," or neutrons in thermal equilibrium with matter at room temperature, possess energies of the right order of magnitude to diffract appreciably from single crystals. Neutrons produced in a nuclear reactor are far too energetic to produce diffraction from crystals and must be slowed down in a graphite column as they leave the reactor. In the graphite moderator, repeated collisions with carbon atoms ultimately reduce the average neutron energies to the average thermal energy of the carbon atoms. When this occurs, these so-called thermalized neutrons possess a distribution of velocities and a corresponding distribution of de Broglie wavelengths with average wavelengths comparable to crystal spacings.

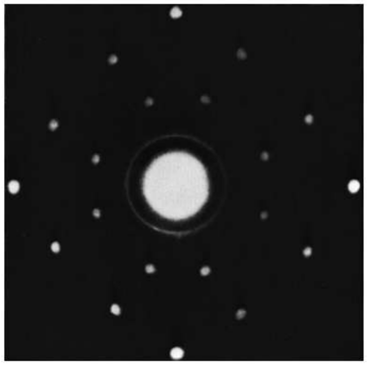


Figure 5-11 Neutron Laue pattern of NaCl. Compare this with the x-ray Laue pattern in Figure 3-14. [*Courtesy of E. O. Wollan and C. G. Shull.*]

Electrons are about 2,000 times lighter than neutrons, to have a wavelength that is suitable for diffraction on crystals, they need to have the same (or more) momentum as these neutrons, i.e. much higher speeds, in electron microscopes they are at relativistic speeds

$$E^2 = (pc)^2 + (mc^2)^2 \qquad \textbf{2-31}$$

Writing E_0 for the rest energy mc^2 of the particle for convenience, this becomes

$$E^2 = (pc)^2 + E_0^2 \qquad \textbf{5-8}$$

Since the total energy $E = E_0 + E_k$, Equation 5-8 becomes

$$(E_0 + E_k)^2 = (pc)^2 + E_0^2$$

that, when solved for p, yields

$$p = \frac{(2E_0E_k + E_k^2)^{1/2}}{c}$$

from which de Broglie equation for special relativity

$$\lambda = \frac{hc}{(2E_0E_k + E_k^2)^{1/2}} \qquad \textbf{5-9}$$

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

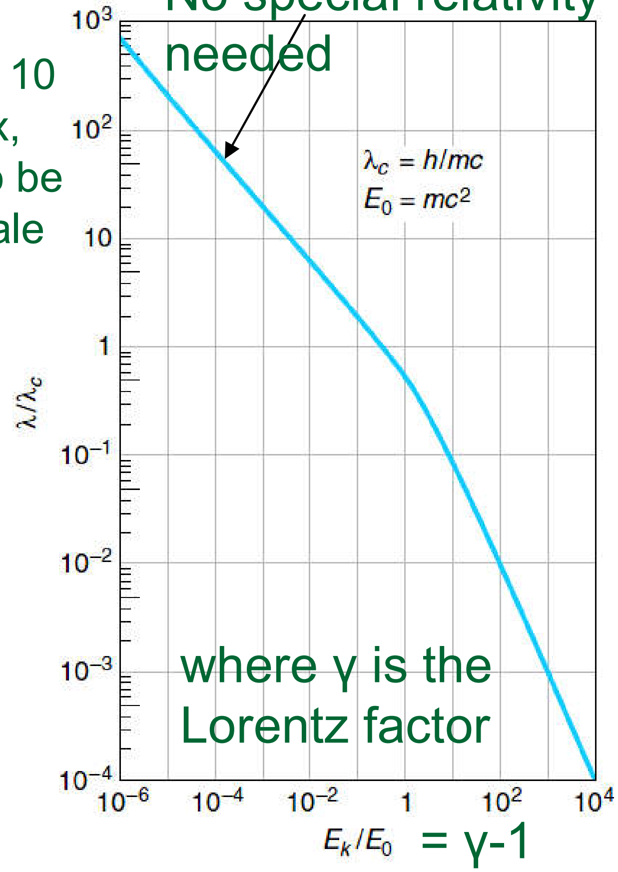
This can be written in a particularly useful way applicable to any particle of any energy by dividing the numerator and denominator by the rest energy $E_0 = mc^2$ as follows:

$$\lambda = \frac{hc/mc^2}{(2E_0E_k + E_k^2)^{1/2}/E_0} = \frac{h/mc}{[2(E_k/E_0) + (E_k/E_0)^2]^{1/2}}$$

Recognizing h/mc as the Compton wavelength λ_c of the particle of mass m (see Section 3-4), we have that, for any particle,

$$\lambda/\lambda_c = \frac{1}{[2(E_k/E_0) + (E_k/E_0)^2]^{1/2}}$$

Note the scaling in powers of 10 on y and x, could also be a $\log_{10}$ scale



No special relativity needed

where γ is the Lorentz factor

= γ-1

Figure 5-13 The de Broglie wavelength λ expressed in units of the Compton wavelength λ_c for a particle of mass m versus the kinetic energy of the particle E_k expressed in units of its rest energy $E_0 = mc^2$. For protons and neutrons $E_0 = 0.938$ GeV and $\lambda_c = 1.32$ fm. For electrons $E_0 = 0.511$ MeV and $\lambda_c = 0.00234$ nm.

an alternative formula for the de Broglie wavelength derived from special relativity and insights from the analysis of the Compton experiment

Rutherford's α-particles had energies on the order of magnitude 5 MeV, experiments are now done with GeV particles, so 200 times more energy

Will they behave "more like" bullets or waves?

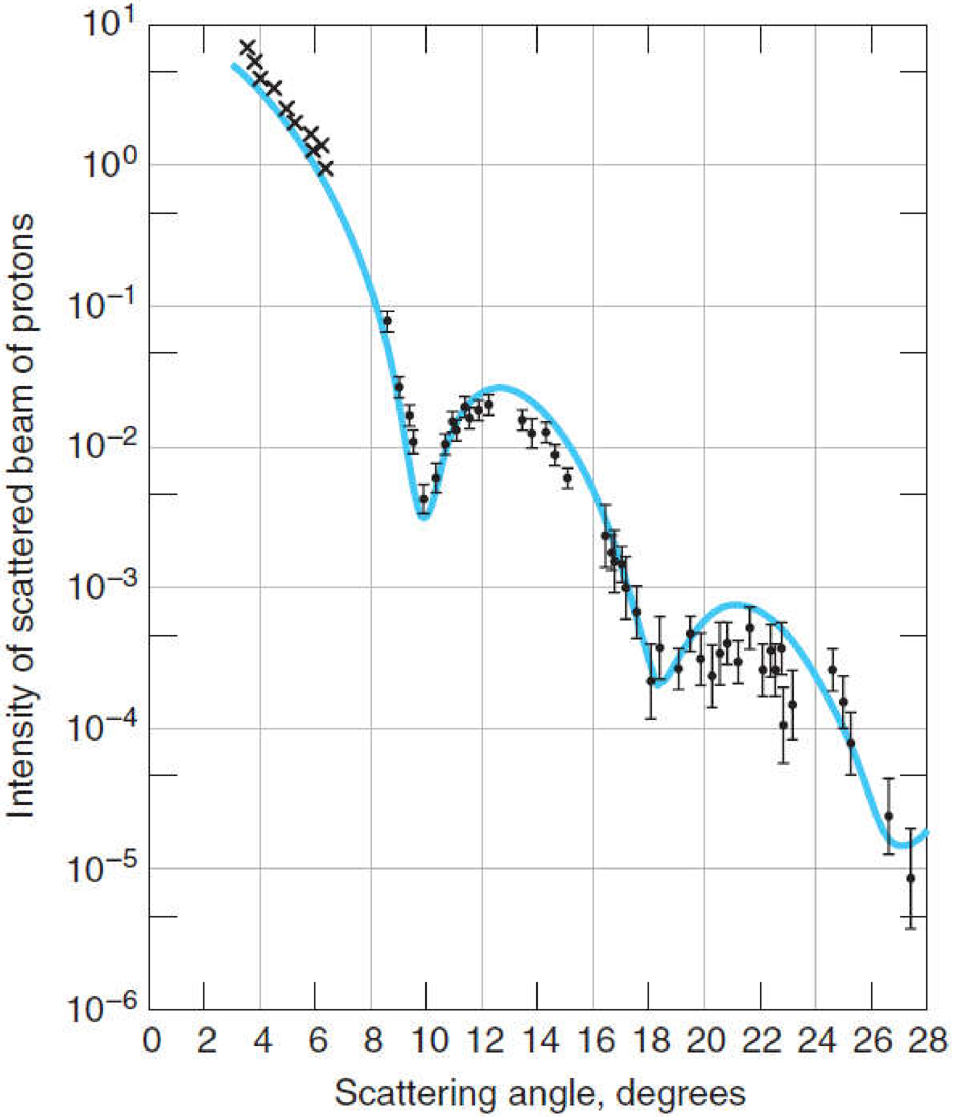


Figure 5-12 Nuclei provide scatterers whose dimensions are of the order of 10^{-15} m. Here the diffraction of 1-GeV protons from oxygen nuclei result in a pattern similar to that of a single slit.

So protons of sufficiently high energy are diffracted by the internal structure of the nuclei, the higher the energy the smaller the length scale

5.4: Wave Motion

- Classical waves and light can be represented by a wave function. A 1D sinusoidal wave traveling to the right (positive x-axis) with time is represented by

$$\Psi(x,t) = A\sin\left[\frac{2\pi}{\lambda}(x - vt)\right]$$

expression in [ ] must be dimensionless

- This is a solution to the wave equation (time dependent Helmholtz equation in Europe)

$$\frac{\partial^2\Psi}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2\Psi}{\partial t^2}$$

The really great thing is that any wave needs to be a solution to this equation, can be derived from Newton's laws in case of classical waves

- Define the wave number *k* and the angular frequency *ω* as:

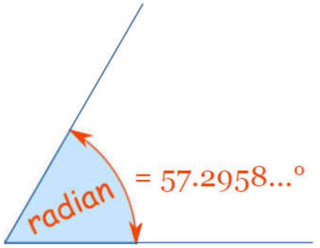
Wave-number $k \equiv \frac{2\pi}{\lambda}$ and $\omega = \frac{2\pi}{T}$ Angular frequency

- The wave function is now: $\Psi(x, t) = A \sin(kx - \omega t)$.

$$y(x,t) = y_0\cos(kx - \omega t) = y_0\cos 2\pi\left(\frac{x}{\lambda} - \frac{t}{T}\right) = y_0\cos\frac{2\pi}{\lambda}(x - vt)$$

Wave Properties

- The phase velocity is the velocity of a point on the wave that has a given phase (for example, the crest) and is given by



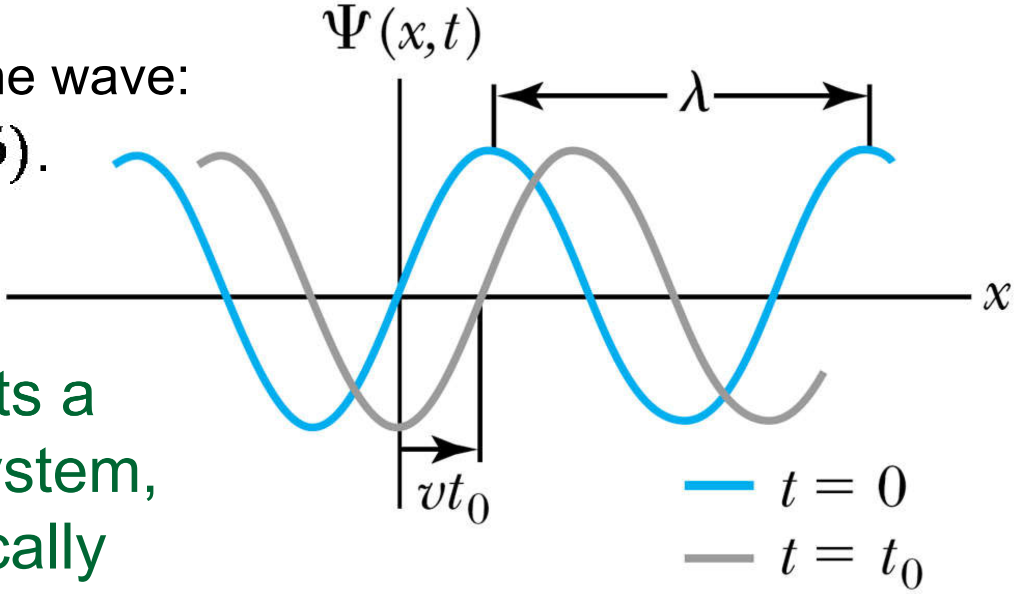
$$v_{\mathrm{ph}} = \frac{\lambda}{T} = \frac{\omega}{k}$$

$\omega = 2\pi f$

- A phase constant Φ shifts the wave:

$$\Psi(x,t) = A\sin(kx - \omega t + \phi).$$

Φ in radian, 360° = 2π rad



A sinusoidal wave represents a free particle, not part of a system, not bound to anything, basically the only particle in the whole of the universe, a model, but good approximation for many purposes

Phase shift of π/2 changes sine into cosine

$\Psi_1(x, t) = A \sin (kx - \omega t)$

$+ \quad \Psi_2 (x, t) = A \cos (kx - \omega t)$

are both solutions to

$$\frac{\partial^2 \Psi}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 \Psi}{\partial t^2}$$

$\Psi_{1+2} (x, t) = A \{\cos (kx - \omega t) + \sin (kx - \omega t)\}$

Since this is a linear equation, the sum of two solutions will also be a solution, constant factors do not matter either

That's all fine for traveling classical waves and light, but

$$e^{i(kx-\omega t)} = \cos(kx - \omega t) + i \sin(kx - \omega t)$$

$\Psi_{\text{complex}} (x, t) = A \{\cos (kx - \omega t) + i \sin (kx - \omega t)\}$ solves both the time dependent Helmholtz equation and the Schrödinger equation which is in its time dependent form also complex (and linear as well), next section of the course, quick glance

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + V\Psi(x,t) \qquad i = \sqrt{-1}$$

Wave function for traveling matter waves need to be complex, standing matter waves are real by superposition

Principle of Superposition of waves

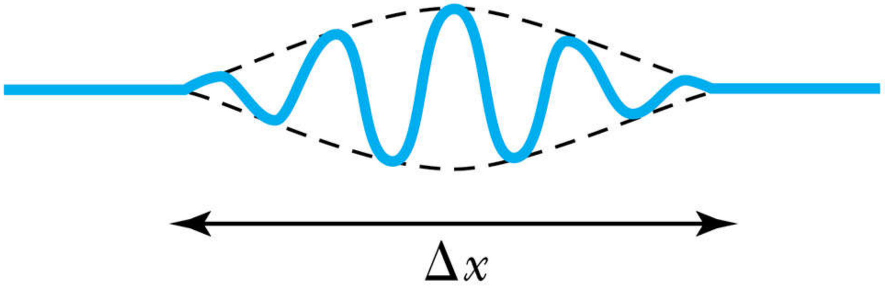
- When two or more waves traverse the same region, they act independently of each other.
- Combining two cos waves with very similar frequency and wave number yield

$$\Psi(x,t) = \Psi_1(x,t) + \Psi_2(x,t) = 2A\overset{\text{cos}}{\searrow}\left(\frac{\Delta k}{2}x - \frac{\Delta\omega}{2}t\right)\cos(k_{\text{av}}x - \omega_{\text{av}}t)$$

- When many more waves are combined, the phase of the wave oscillates within an envelope that denotes the maximum displacement of the combined waves.
- When combining (infinitely many) waves with different amplitudes and frequencies and wave numbers, a pulse, or **wave packet**, is formed which moves at a **group velocity**:

$$u_{\text{gr}} = \Delta\omega / \Delta k.$$

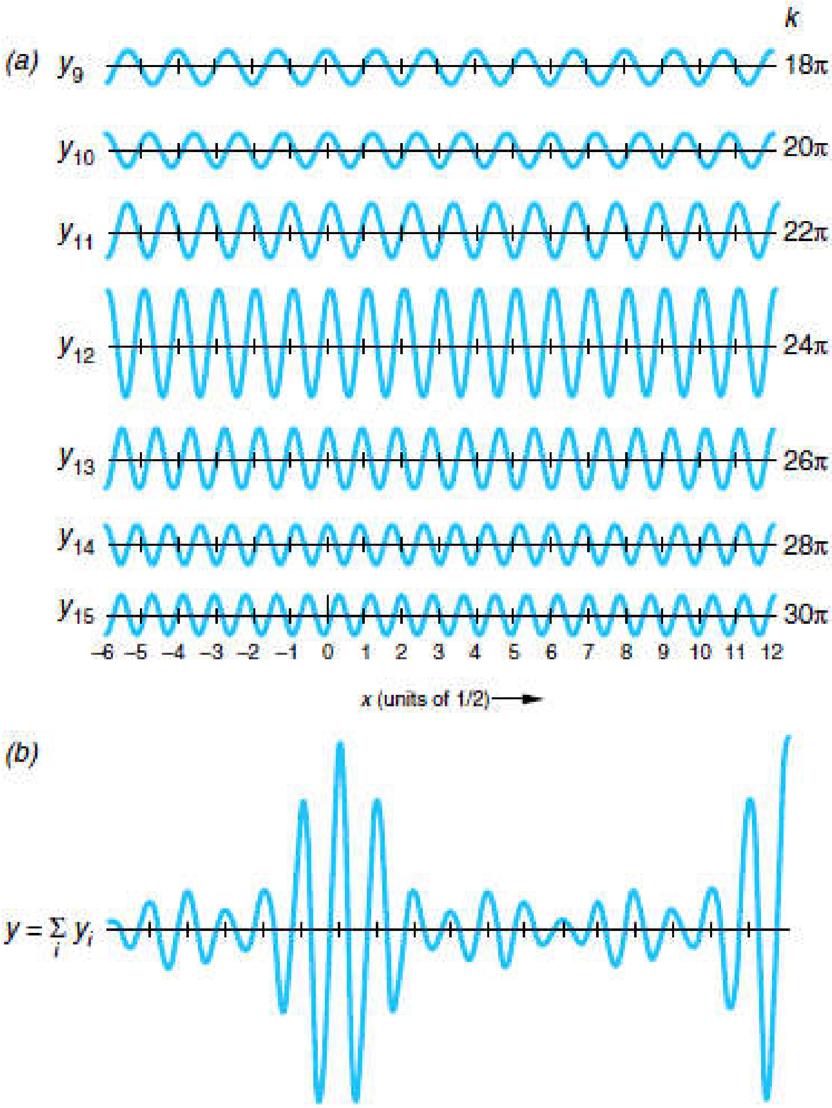
Superimposing many many different sinusoidal waves



Details in the following slides

y is just amplitude, not a space dimension, as we have a 1D wave (x,t)

Superposition of many different sinusoidal waves to a blob, which represents a particle, this blob travels with the group velocity = velocity of the particle that it represents



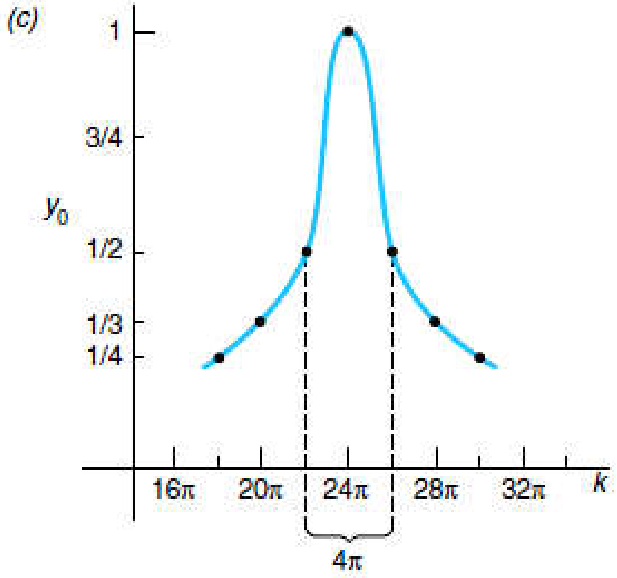


Figure 5-16 (a) Superposition of seven sinusoids $y_k(x, t) = y_{0k} \cos(kx - \omega t)$ with uniformly spaced wave numbers ranging from $k = (2\pi)9$ to $k = (2\pi)15$ with $t = 0$. The maximum amplitude is 1 at the center of the range ($k = (2\pi)12$), decreasing to 1/2, 1/3, and 1/4, respectively, for the waves on each side of the central wave. (b) The sum $y(x, 0) = \sum_{i=9}^{15} y_i(x, 0)$ is maximum at $x = 0$ with additional maxima equally spaced along the ±x axis. (c) Amplitudes of the sinusoids y_i versus wave number k.

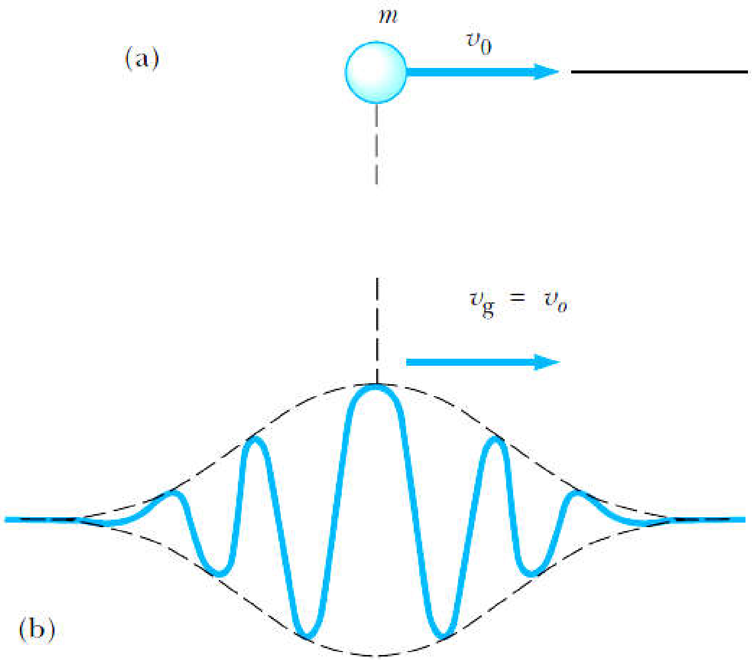


Figure 5.17 Representing a particle with matter waves: (a) particle of mass m and speed v_0; (b) superposition of many matter waves with a spread of wavelengths centered on $\lambda_0 = h/mv_0$ correctly represents a particle.

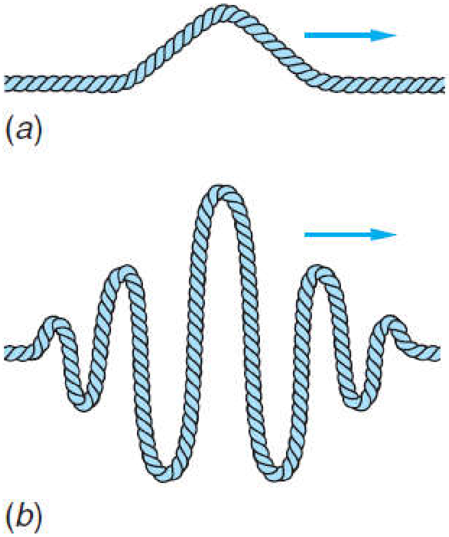


Figure 5-14 (*a*) Wave pulse moving along a string. A pulse has a beginning and an end; i.e., it is localized, unlike a pure harmonic wave, which goes on forever in space and time. (*b*) A wave packet formed by the superposition of harmonic waves.

Group velocity and phase velocity are different, a wave group moves with the group velocity – which de Broglie showed to be the same as the velocity of the particle v_0

The waves that form the pulse have a wide range of phase velocities, wave numbers, intensities, angular frequencies.

Phenomena of beats, two superimposed waves

$$y(x,t) = y_0\cos(k_1x - \omega_1t) + y_0\cos(k_2x - \omega_2t) \rightarrow y(x,t) = 2y_0\cos\left(\frac{\Delta k}{2}x - \frac{\Delta\omega}{2}t\right)\cos\left(\frac{k_1+k_2}{2}x - \frac{\omega_1+\omega_2}{2}t\right)$$

$$y(x,t)) = 2y_0\cos\left(\frac{1}{2}\Delta kx - \frac{1}{2}\Delta\omega t\right)\cos(\bar{k}x - \bar{\omega}t)$$

$\Delta k = k_2 - k_1$

$\Delta\omega = \omega_2 - \omega_1$

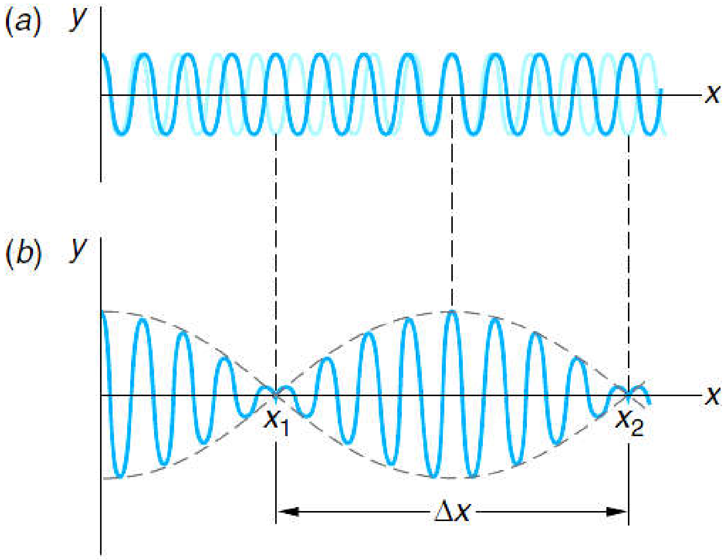
small if waves are similar

$\bar{\omega} = (\omega_1 + \omega_2)/2$

$\bar{k} = (k_1 + k_2)/2$

large if waves are similar

The wave within the envelope moves with the speed $\bar{\omega}/\bar{k}$, the phase velocity v_p due to the second cosine term. If we write the first (amplitude-modulating) term as $\cos\{\frac{1}{2}\Delta k[x - (\Delta\omega/\Delta k)\,t]\}$, we see that the envelope moves with speed $\Delta\omega/\Delta k$. The speed of the envelope is called the *group velocity* v_g.



$$v_p = \frac{(\omega_1+\omega_2)/2}{(k_1+k_2)/2} \approx \frac{\omega_1}{k_1} = v_1$$

$$v_g = \frac{(\omega_2-\omega_1)/2}{(k_2-k_1)/2} = \frac{\Delta\omega}{\Delta k}$$

high

low

Figure 5-15 Two waves of slightly different wavelength and frequency produce beats. (*a*) Shows $y(x)$ at a given instant for each of the two waves. The waves are in phase at the origin, but because of the difference in wavelength, they become out of phase and then in phase again. (*b*) The sum of these waves. The spatial extent of the group Δx is inversely proportional to the difference in wave numbers Δk, where k is related to the wavelength by $k = 2\pi/\lambda$. Identical figures are obtained if y is plotted versus time t at a fixed point x. In that case the extent in time Δt is inversely proportional to the frequency difference $\Delta\omega$.

Mathematical uncertainty principle for the scenario of beats

$$y(x, t)) = 2y_0 \cos\left(\frac{1}{2}\Delta k x - \frac{1}{2}\Delta\omega t\right)\cos(\bar{k}x - \bar{\omega}t)$$

Note that this is a function of 2 variables

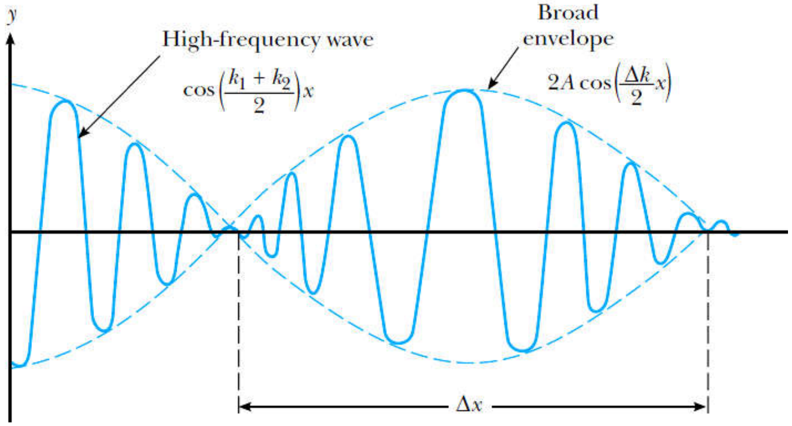
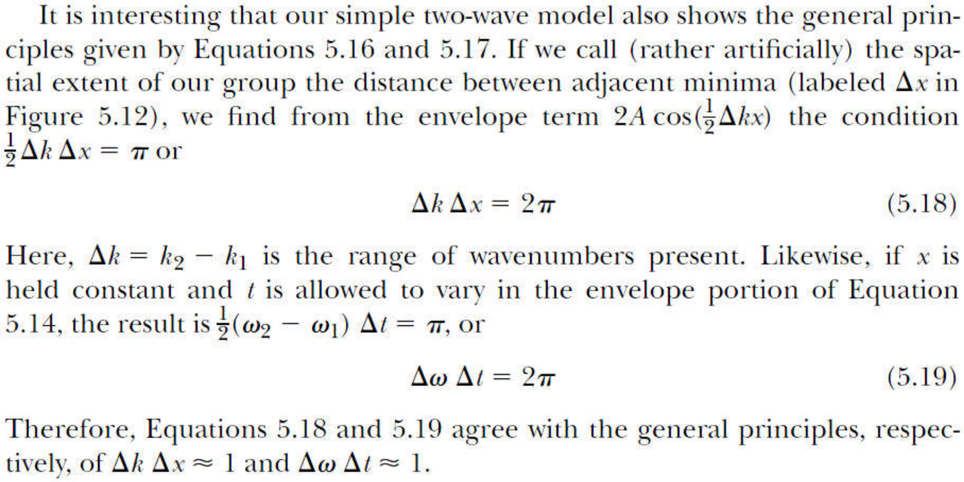


Figure 5.19 Superposition of two waves of slightly different wavelengths resulting in primitive wave groups; t has been set equal to zero in Equation 5.14.


It is interesting that our simple two-wave model also shows the general principles given by Equations 5.16 and 5.17. If we call (rather artificially) the spatial extent of our group the distance between adjacent minima (labeled Δx in Figure 5.12), we find from the envelope term $2A\cos(\frac{1}{2}\Delta kx)$ the condition $\frac{1}{2}\Delta k\,\Delta x = \pi$ or

$$\Delta k\,\Delta x = 2\pi \qquad (5.18)$$

Here, $\Delta k = k_2 - k_1$ is the range of wavenumbers present. Likewise, if x is held constant and t is allowed to vary in the envelope portion of Equation 5.14, the result is $\frac{1}{2}(\omega_2 - \omega_1)\,\Delta t = \pi$, or

$$\Delta\omega\,\Delta t = 2\pi \qquad (5.19)$$

Therefore, Equations 5.18 and 5.19 agree with the general principles, respectively, of $\Delta k\,\Delta x \approx 1$ and $\Delta\omega\,\Delta t \approx 1$.

For infinitely many waves with enormously range of frequencies and wave numbers, we get these mathematical uncertainties

$$\Delta x\,\Delta k \approx 1 \qquad \lambda = \frac{h}{p}$$ de Broglie

$$\Delta t\,\Delta\omega \approx 1 \qquad f = \frac{E}{h}$$ Planck-Einstein

5.4 FOURIER INTEGRALS

In this section we show in detail how to construct wave groups, or pulses, that are truly localized in space or time and also show that very general reciprocity relations of the type $\Delta k \Delta x \approx 1$ and $\Delta\omega\Delta t \approx 1$ hold for these pulses.

To form a true pulse that is zero everywhere outside of a finite spatial range Δx requires adding together an infinite number of harmonic waves with continuously varying wavelengths and amplitudes. This addition can be done with a Fourier integral, which is defined as follows:

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} a(k)\, e^{ikx} dk \tag{5.26}$$

Here $f(x)$ is a spatially localized wave group, $a(k)$ gives the amount or amplitude of the wave with wavenumber $k = (2\pi/\lambda)$ to be added, and $e^{ikx} = \cos kx + i \sin kx$ is Euler's compact expression for a harmonic wave. The amplitude distribution function $a(k)$ can be obtained if $f(x)$ is known by using the symmetric formula

$\Delta k_x \cdot \Delta x \approx 1$

$$a(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x)\, e^{-ikx} dx \tag{5.27}$$

- Loosely speaking,

- These integrals are reciprocal-”symmetric” to each other, obviously e^x times $e^{-x} = e^0 = 1$
- because f(x) and a(k) are reciprocal to each other we speak of direct or physical space and reciprocal of Fourier space (sometimes diffraction space)

https://www.youtube.com/watch?v=MBnnXbOM5S4

A mixture of maths+physics+entertainment, a whole visual series:
3Blue1Brown channel

Visualization Fourier transform:
https://www.youtube.com/watch?v=spUNpyF58BY&t=12s

Fourier series
https://www.youtube.com/watch?v=r6sGWTCMz2k

Equations 5.26 and 5.27 apply to the case of a spatial pulse at fixed time, but it is important to note that they are mathematically identical to the case of a time pulse passing a fixed position. This case is common in electrical engineering and involves adding together a continuously varying set of frequencies:

$$V(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} g(\omega) e^{i\omega t} d\omega \tag{5.28}$$

$$g(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} V(t) e^{-i\omega t} dt \tag{5.29}$$

where $V(t)$ is the strength of a signal as a function of time, and $g(\omega)$ is the *spectral content* of the signal and gives the amount of the harmonic wave with frequency ω that is present.

$$\Delta\omega \cdot \Delta t \approx 1$$

$\Delta x \cdot \Delta k \approx 1$ multiply with $\hbar$

$\Delta x \cdot \Delta k \cdot \hbar \approx \hbar$ what is $\Delta k \cdot \hbar$? it is actually Δp why?

because $k = \frac{2\pi}{\lambda}$ and with de Broglie $p = \hbar k$

leading by differentiation and expansion to deltas $\Delta p = \hbar \Delta k$ so $\Delta x \cdot \Delta p \approx \hbar$

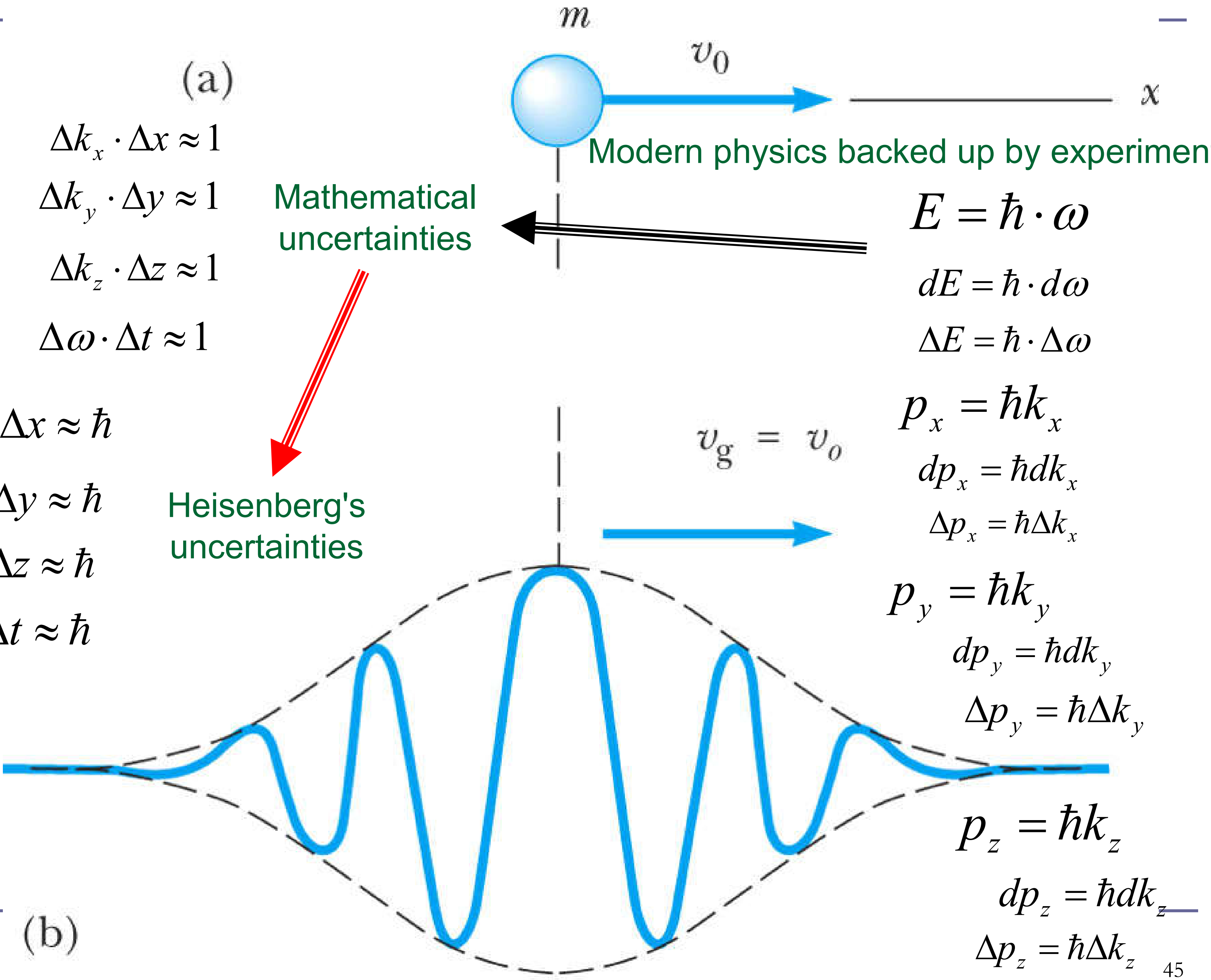
$\Delta t \cdot \Delta \omega \approx 1$ multiply with $\hbar$

$\Delta t \cdot \Delta \omega \cdot \hbar \approx \hbar$ what is $\Delta \omega \cdot \hbar$? it is actually ΔE why? , because

$\omega = 2\pi \cdot f$ and with Plank-Einstein $E = \hbar \omega$

leading by differentiation and expansion to deltas $\Delta E = \hbar \Delta \omega$ so $\Delta t \cdot \Delta E \approx \hbar$

GREAT out of two mathematical uncertainties, we derived by physical interpretation of a matter wave pulse (using de Broglie and Planck-Einstein) Heisenberg's uncertainty principle



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$$\Delta k_x \cdot \Delta x \approx 1$$
$$\Delta k_y \cdot \Delta y \approx 1$$
$$\Delta k_z \cdot \Delta z \approx 1$$
$$\Delta \omega \cdot \Delta t \approx 1$$

Mathematical uncertainties

$$\Delta p_x \cdot \Delta x \approx \hbar$$
$$\Delta p_y \cdot \Delta y \approx \hbar$$
$$\Delta p_z \cdot \Delta z \approx \hbar$$
$$\Delta E \cdot \Delta t \approx \hbar$$

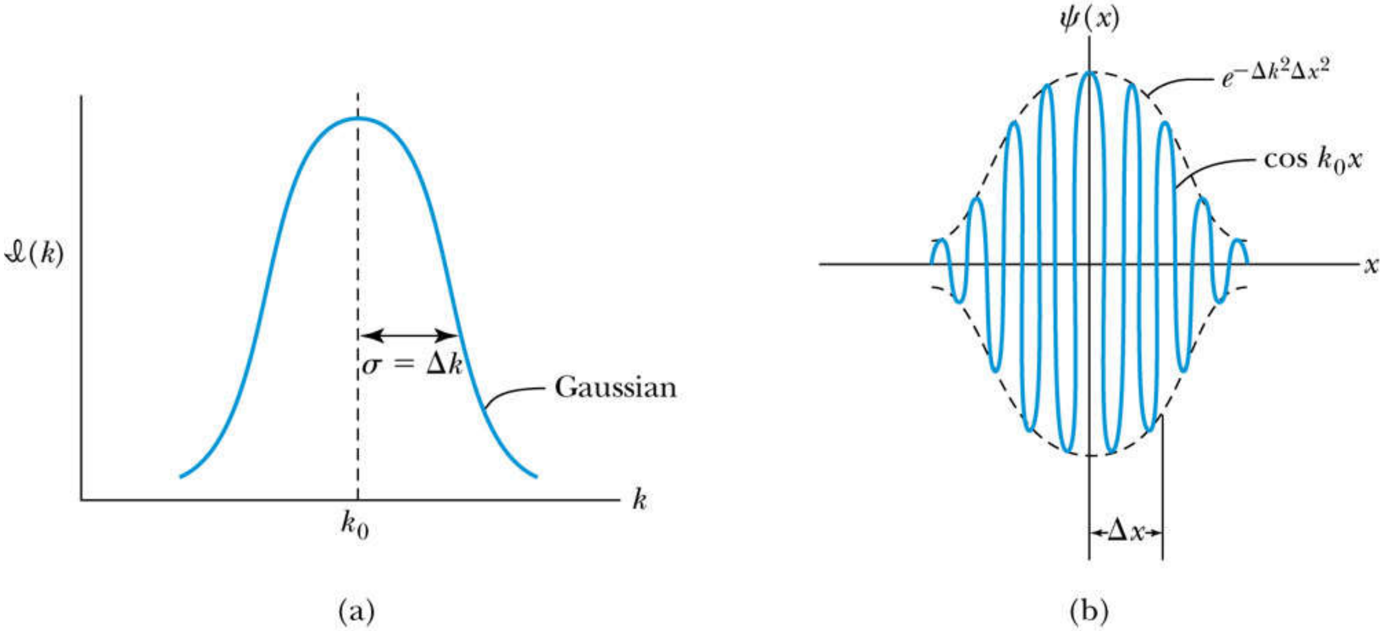
Heisenberg's uncertainties

Modern physics backed up by experiments

$$E = \hbar \cdot \omega$$
$$dE = \hbar \cdot d\omega$$
$$\Delta E = \hbar \cdot \Delta \omega$$
$$p_x = \hbar k_x$$
$$dp_x = \hbar dk_x$$
$$\Delta p_x = \hbar \Delta k_x$$
$$p_y = \hbar k_y$$
$$dp_y = \hbar dk_y$$
$$\Delta p_y = \hbar \Delta k_y$$
$$p_z = \hbar k_z$$
$$dp_z = \hbar dk_z$$
$$\Delta p_z = \hbar \Delta k_z$$

Gaussian Function and wave packet

- A Gaussian wave packet may approximate the envelope of a certain pulse wave. $\Psi(x,0) = \Psi(x) = Ae^{-\Delta k^2 x^2}\cos(k_0 x)$



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- The group velocity is $u_{\rm gr} = \dfrac{d\omega}{dk}$.

Fourier transform of Gaussian or normal distribution function, (zero mean and standard deviation σ).

$$f(t) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{t^2}{2\sigma^2}\right) \qquad -\infty < t < \infty$$

$$\text{thus} \quad g(\omega) = (2\pi\sigma)^{-1} \int_{-\infty}^{\infty} \exp(-t^2/2\sigma^2)\exp(-i\omega t)\,dt$$

$$= (2\pi\sigma)^{-1} \int_{-\infty}^{\infty} \exp\left[-\frac{1}{2\sigma^2}\left(t^2 + 2\sigma^2 i\omega t + (\sigma^2 i\omega)^2 - (\sigma^2 i\omega)^2\right)\right] dt$$

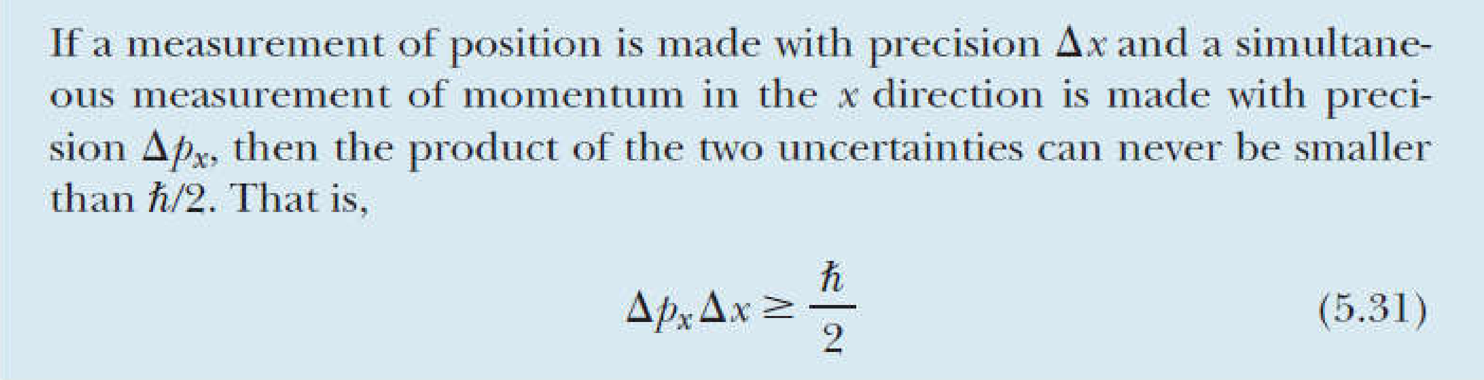
which can be rewritten as $$g(\omega) = \frac{\exp(-\sigma^2\omega^2/2)}{\sqrt{2\pi}} \frac{1}{\sigma\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left[-\frac{(t + i\sigma^2\omega)^2}{2\sigma^2}\right] dt$$

Finally this can be shown to give $$g(\omega) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\sigma^2\omega^2}{2}\right)$$

which is also a Gaussian distribution with zero mean but with standard deviation equal to 1/σ, i.e. **$\sigma_\omega \sigma_t = 1$**

The narrower in time a pulse is, the greater the spread of its frequency components. That's again the mathematical uncertainty principle.

for the ideal of a Gaussian wave packet only



If a measurement of position is made with precision Δx and a simultaneous measurement of momentum in the x direction is made with precision Δp_x, then the product of the two uncertainties can never be smaller than $\hbar/2$. That is,

$$\Delta p_x \Delta x \geq \frac{\hbar}{2} \qquad (5.31)$$

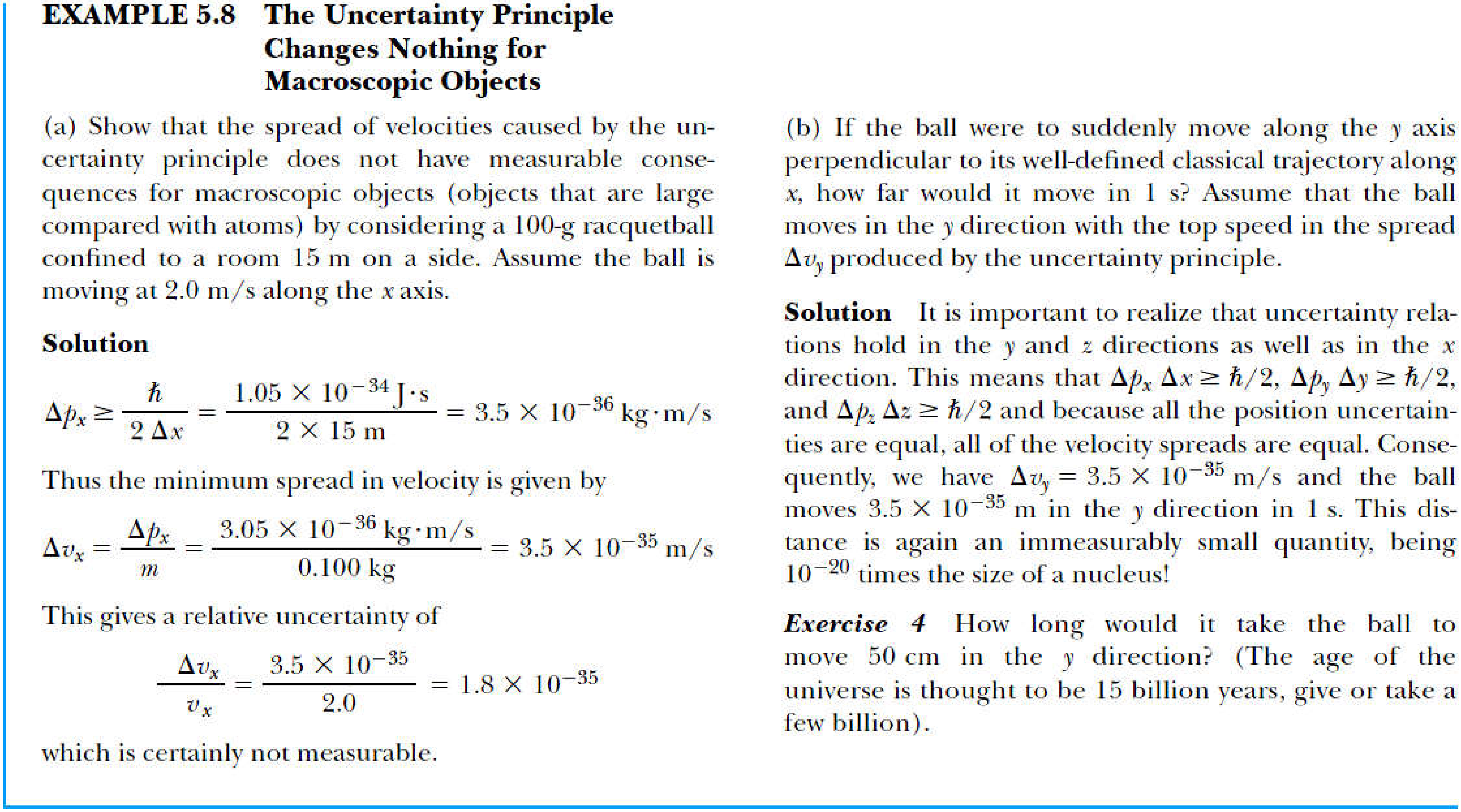
There can be three components of vector p in 3D, so three times (5.31)

The uncertainty principle has actually nothing to do with measurements, repeated measurements won't do you any good, it is loosely speaking a **systematic rest error** that nobody can correct, just nature is at the quantum level a bit fuzzy, doesn't behave as we are used to from classical physics for large objects.

Energy–time uncertainty principle

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

Given for one instant an intelligence which could comprehend all the forces by which nature is animated and the respective positions of the things which compose it...nothing would be uncertain, and the future as the past would be laid out before its eyes. *Pierre Simon de Laplace, 1776*



EXAMPLE 5.8 The Uncertainty Principle Changes Nothing for Macroscopic Objects

(a) Show that the spread of velocities caused by the uncertainty principle does not have measurable consequences for macroscopic objects (objects that are large compared with atoms) by considering a 100-g racquetball confined to a room 15 m on a side. Assume the ball is moving at 2.0 m/s along the *x* axis.

Solution

$$\Delta p_x \geq \frac{\hbar}{2\,\Delta x} = \frac{1.05 \times 10^{-34}\ \mathrm{J \cdot s}}{2 \times 15\ \mathrm{m}} = 3.5 \times 10^{-36}\ \mathrm{kg \cdot m/s}$$

Thus the minimum spread in velocity is given by

$$\Delta v_x = \frac{\Delta p_x}{m} = \frac{3.05 \times 10^{-36}\ \mathrm{kg \cdot m/s}}{0.100\ \mathrm{kg}} = 3.5 \times 10^{-35}\ \mathrm{m/s}$$

This gives a relative uncertainty of

$$\frac{\Delta v_x}{v_x} = \frac{3.5 \times 10^{-35}}{2.0} = 1.8 \times 10^{-35}$$

which is certainly not measurable.

(b) If the ball were to suddenly move along the *y* axis perpendicular to its well-defined classical trajectory along *x*, how far would it move in 1 s? Assume that the ball moves in the *y* direction with the top speed in the spread Δv_y produced by the uncertainty principle.

Solution It is important to realize that uncertainty relations hold in the *y* and *z* directions as well as in the *x* direction. This means that $\Delta p_x\,\Delta x \geq \hbar/2$, $\Delta p_y\,\Delta y \geq \hbar/2$, and $\Delta p_z\,\Delta z \geq \hbar/2$ and because all the position uncertainties are equal, all of the velocity spreads are equal. Consequently, we have $\Delta v_y = 3.5 \times 10^{-35}$ m/s and the ball moves 3.5×10^{-35} m in the *y* direction in 1 s. This distance is again an immeasurably small quantity, being 10^{-20} times the size of a nucleus!

Exercise 4 How long would it take the ball to move 50 cm in the *y* direction? (The age of the universe is thought to be 15 billion years, give or take a few billion).

One billion years ≈ 3.154 10^{16} seconds

Probability of finding a particle at a certain point in space and time, modification of same slide will be shown later on again

- The “square” of wave function determines the likelihood (or probability) of finding a particle at a particular position in space at a given time.

$$P(y)\,dy = \left|\Psi(y,t)\right|^2\,dy$$

- The total probability of finding the electron is 1 (or 100%). Forcing this condition on the wave function is called normalization.

$$\int_{-\infty}^{\infty} P(y)\,dy = \int_{-\infty}^{\infty} \left|\Psi(y,t)\right|^2\,dy = 1$$ If wave function is normalized !!

$$\int_{-\infty}^{\infty} \Psi^*(y,t)\cdot\Psi(y,t)\cdot dy = something \quad \Psi_{normalized}(y,t) = {}^{1}\!\big/\!\sqrt{something}\;\Psi(y,t)$$

dy for no particular reason, it’s just 1D *dx,* (in 3D space with time separated (not 4D) as the particle doesn’t move very fast)

Probability and square of Wave Function

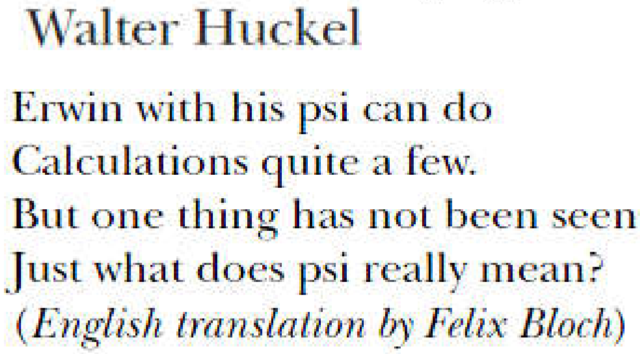
- The square of wave function determines the likelihood (or probability) of finding a particle at a particular position in space at a given time.

$$P(y)\,dy = \left|\Psi(y,t)\right|^2\,dy$$

dy for no particular reason, it's just 1D *dx*

- The total probability of finding the electron is 100%. Forcing this condition on the wave function is called normalization.

$$\int_{-\infty}^{\infty} P(y)\,dy = \int_{-\infty}^{\infty} \left|\Psi(y,t)\right|^2\,dy = 1$$



Walter Huckel

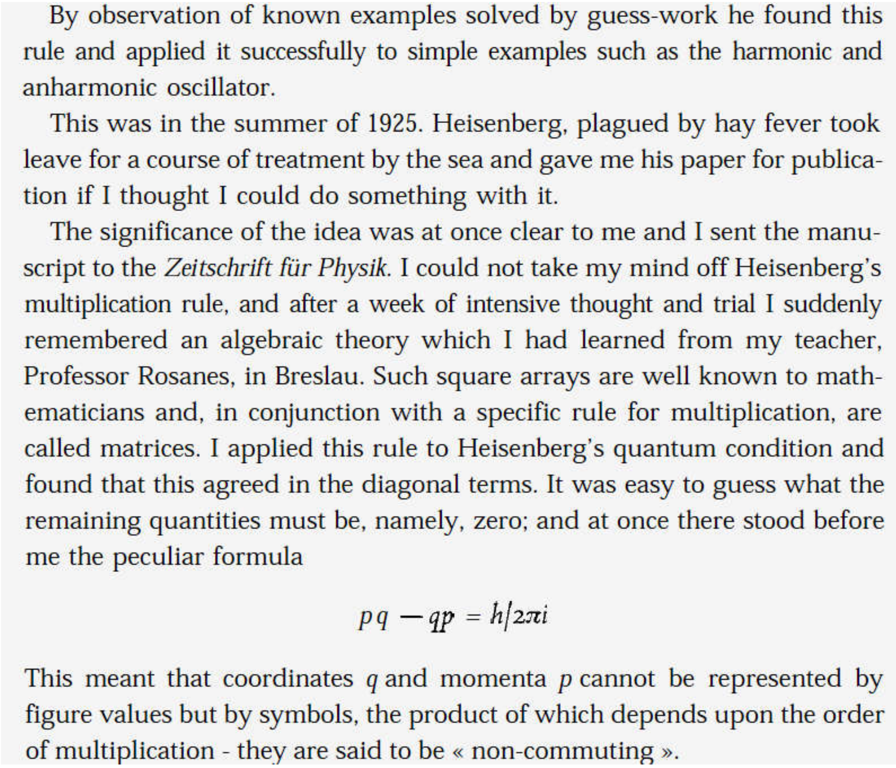
Erwin with his psi can do
Calculations quite a few.
But one thing has not been seen
Just what does psi really mean?
(*English translation by Felix Bloch*)

Nobel Prize 1954 to Max Born: “*"for his fundamental research in quantum mechanics, especially for his statistical interpretation of the wave function"*

Normalization sets a scale to all further calculations …

$$pq - qp = h/2\pi i$$

“somewhere here” at a cemetery of Göttingen/Germany are the remains of the GREAT Max Born and his lovely wife



By observation of known examples solved by guess-work he found this rule and applied it successfully to simple examples such as the harmonic and anharmonic oscillator.

This was in the summer of 1925. Heisenberg, plagued by hay fever took leave for a course of treatment by the sea and gave me his paper for publication if I thought I could do something with it.

The significance of the idea was at once clear to me and I sent the manuscript to the *Zeitschrift für Physik*. I could not take my mind off Heisenberg's multiplication rule, and after a week of intensive thought and trial I suddenly remembered an algebraic theory which I had learned from my teacher, Professor Rosanes, in Breslau. Such square arrays are well known to mathematicians and, in conjunction with a specific rule for multiplication, are called matrices. I applied this rule to Heisenberg's quantum condition and found that this agreed in the diagonal terms. It was easy to guess what the remaining quantities must be, namely, zero; and at once there stood before me the peculiar formula

$$pq - qp = h/2\pi i$$

This meant that coordinates q and momenta p cannot be represented by figure values but by symbols, the product of which depends upon the order of multiplication - they are said to be « non-commuting ».

Classical physics $pq - qp = 0$

http://www.nobelprize.org/nobel_prizes/physics/laureates/1954/born-lecture.pdf

The art of guessing correct formulae, which deviate from the classical formulae, yet contain them as a limiting case according to the correspondence principle, was brought to a high degree of perfection. A paper of mine, ...

Heisenberg, who at that time was my assistant, brought this period to a sudden end[5]. He cut the Gordian knot by means of a philosophical principle and replaced guess-work by a mathematical rule. The principle states that concepts and representations that do not correspond to physically observable facts are not to be used in theoretical description. Einstein used the

same principle when, in setting up his theory of relativity, he eliminated the concepts of absolute velocity of a body and of absolute simultaneity of two events at different places. Heisenberg banished the picture of electron orbits with definite radii and periods of rotation because these quantities are not observable, and insisted that the theory be built up by means of the square arrays mentioned above. Instead of describing the motion by giving a coordinate as a function of time, *x(t)*, an array of transition amplitudes x_{mn} should be determined. To me the decisive part of his work is the demand to determine a rule by which from a given

array $\begin{bmatrix} x_{11} & x_{12} & \cdots\cdots \\ x_{21} & x_{22} & \cdots\cdots \end{bmatrix}$ the array for the square $\begin{bmatrix} (x^2)_{11} & (x^2)_{12} & \cdots\cdots \\ (x^2)_{21} & (x^2)_{22} & \cdots\cdots \end{bmatrix}$

array $\begin{bmatrix} x_{11} & x_{12} & \cdots\cdots \\ x_{21} & x_{22} & \cdots\cdots \\ - - & - - & - - - - - \end{bmatrix}$ the array for the square $\begin{bmatrix} (x^2)_{11} & (x^2)_{12} & \cdots\cdots \\ (x^2)_{21} & (x^2)_{22} & \cdots\cdots \\ - - - & - - - & - - - - - \end{bmatrix}$

can be found (or, more general, the *multiplication rule* for such arrays). By observation of known examples solved by guess-work he found this rule and applied it successfully to simple examples such as the harmonic and anharmonic oscillator.

This was in the summer of 1925. Heisenberg, plagued by hay fever took leave for a course of treatment by the sea and gave me his paper for publication if I thought I could do something with it.

The significance of the idea was at once clear to me and I sent the manuscript to the *Zeitschrift für Physik*. I could not take my mind off Heisenberg's multiplication rule, and after a week of intensive thought and trial I suddenly remembered an algebraic theory which I had learned from my teacher, Professor Rosanes, in Breslau. Such square arrays are well known to mathematicians and, in conjunction with a specific rule for multiplication, are called matrices. I applied this rule to Heisenberg's quantum condition and found that this agreed in the diagonal terms. It was easy to guess what the remaining quantities must be, namely, zero; and at once there stood before me the peculiar formula

$$pq - qp = h/2\pi i$$

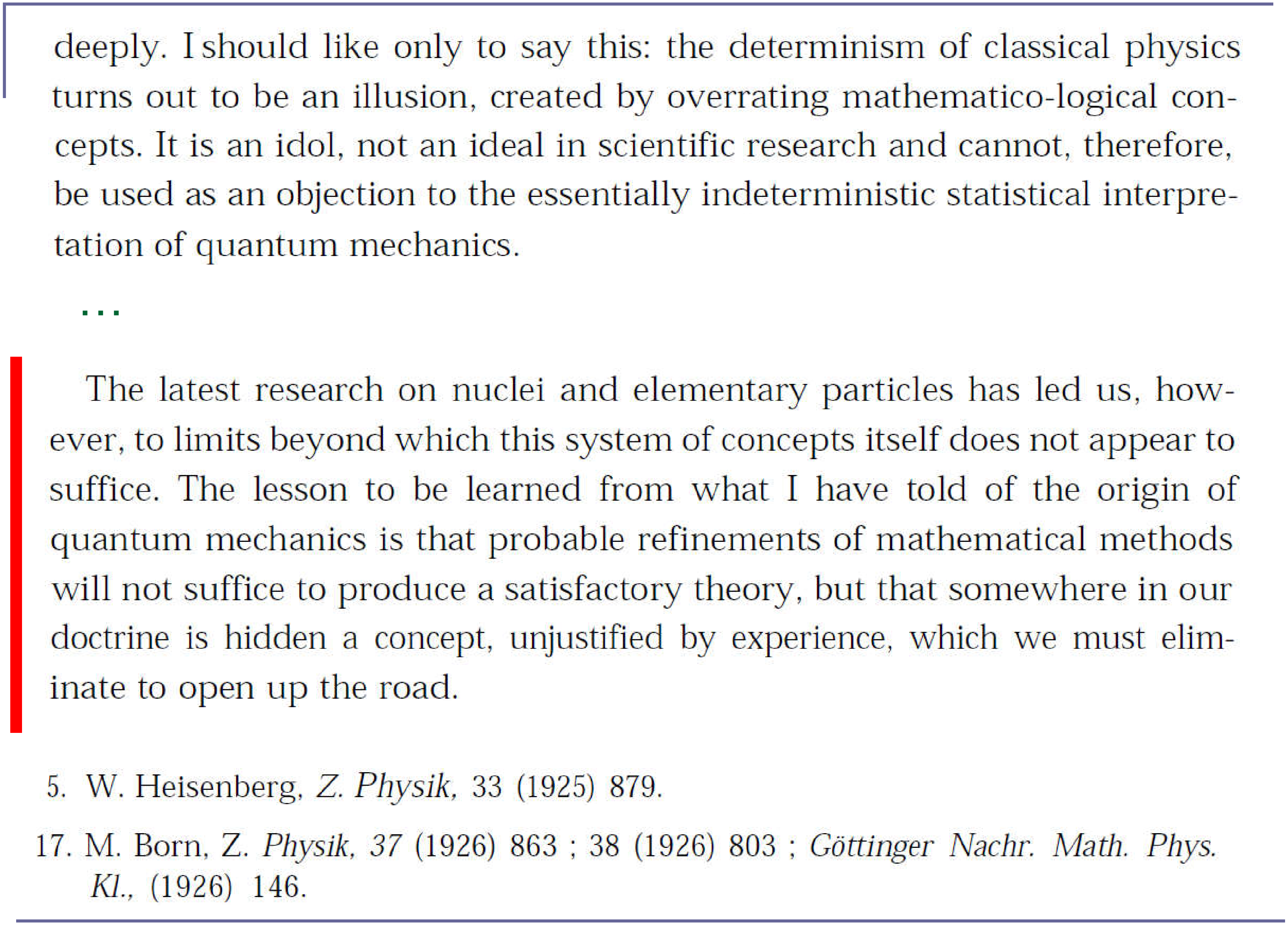
This meant that coordinates q and momenta p cannot be represented by figure values but by symbols, the product of which depends upon the order of multiplication - they are said to be « non-commuting ».

…

This was left to Schrödinger, and I immediately took up his method since it held promise of leading to an interpretation of the ψ-function. Again an idea of Einstein's gave me the lead. He had tried to make the duality of particles - light quanta or photons - and waves comprehensible by interpreting the square of the optical wave amplitudes as probability density for the occurrence of photons. This concept could at once be carried over to the ψ-function: $|\psi|^2$ ought to represent the probability density for electrons (or other particles). It was easy to assert this, but how could it be proved?

… atomic collision processes suggested themselves …

ally, as it is called. In this way it was possible to get a theoretical basis[17] for the assumptions of Bohr's theory which had been experimentally confirmed by Franck and Hertz. Soon Wentzel[18] succeeded in deriving Rutherford's famous formula for the scattering of α-particles from my theory.



deeply. I should like only to say this: the determinism of classical physics turns out to be an illusion, created by overrating mathematico-logical concepts. It is an idol, not an ideal in scientific research and cannot, therefore, be used as an objection to the essentially indeterministic statistical interpretation of quantum mechanics.

…

The latest research on nuclei and elementary particles has led us, however, to limits beyond which this system of concepts itself does not appear to suffice. The lesson to be learned from what I have told of the origin of quantum mechanics is that probable refinements of mathematical methods will not suffice to produce a satisfactory theory, but that somewhere in our doctrine is hidden a concept, unjustified by experience, which we must eliminate to open up the road.

5. W. Heisenberg, *Z. Physik,* 33 (1925) 879.

17. M. Born, *Z. Physik, 37* (1926) 863 ; 38 (1926) 803 ; *Göttinger Nachr. Math. Phys. Kl.,* (1926) 146.

The two Nobel prize papers mentioned above.

Dispersion

- Considering the group velocity of a de Broglie wave packet yields:

$$u_{\mathrm{gr}} = \frac{dE}{dp} = \frac{pc^2}{E}$$

- The relationship between the phase velocity and the group velocity is

$$u_{\mathrm{gr}} = \frac{d\omega}{dk} = \frac{d}{dk}(v_{\mathrm{ph}}k) = v_{\mathrm{ph}} + k\frac{dv_{\mathrm{ph}}}{dk}$$

- Hence the group velocity may be greater or less than the phase velocity. A medium is called nondispersive when the phase velocity is the same for all frequencies and equal to the group velocity.

All matter waves are dispersing – they do not need a medium to travel in, it's simply a consequence of the uncertainty principle, a light pulse in vacuum does not disperse, a light signal in a glass fiber does

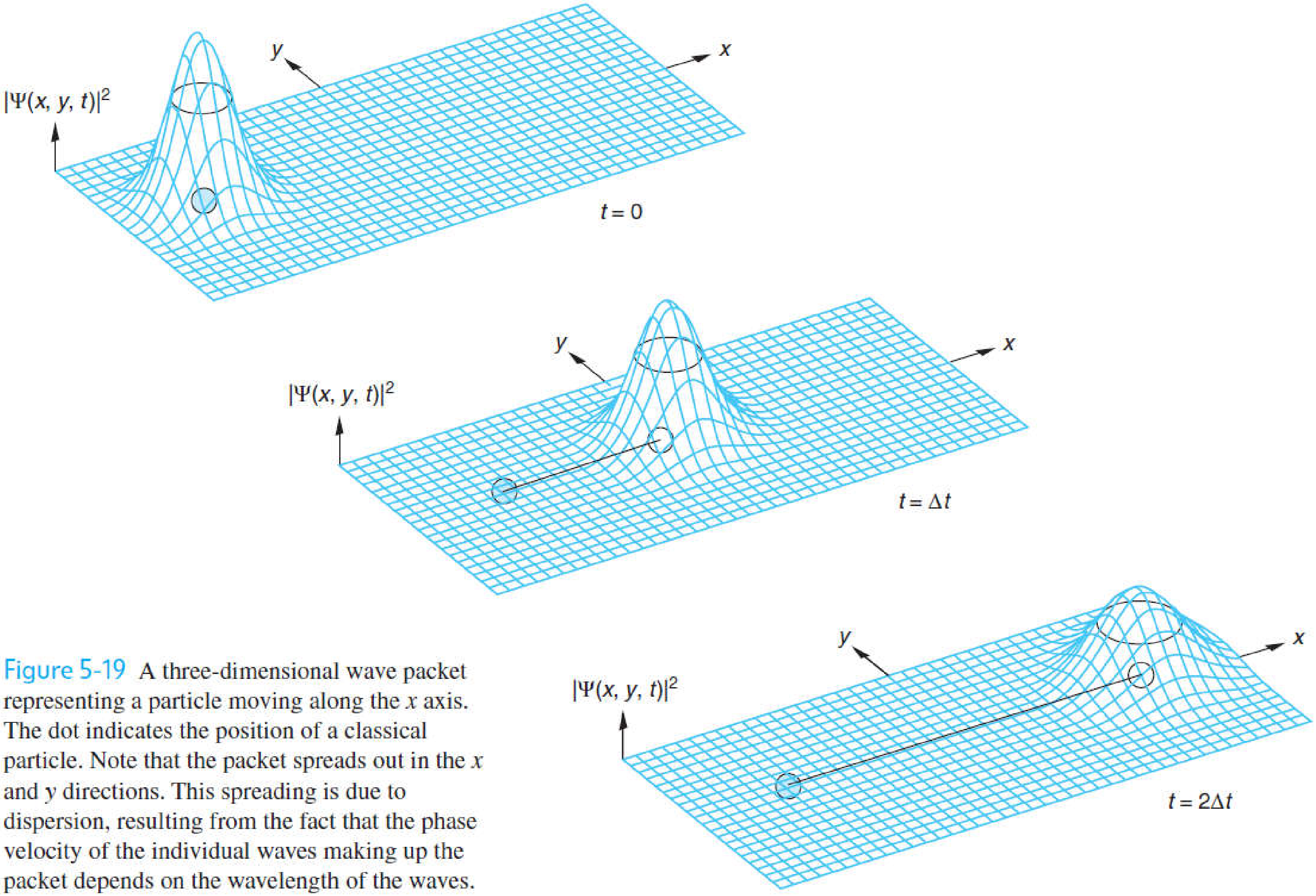
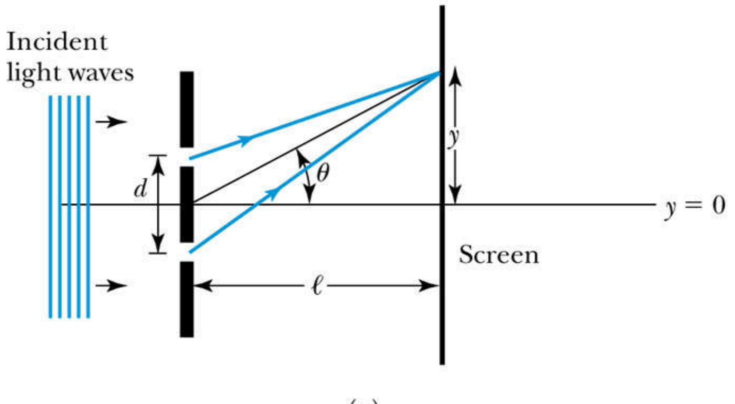


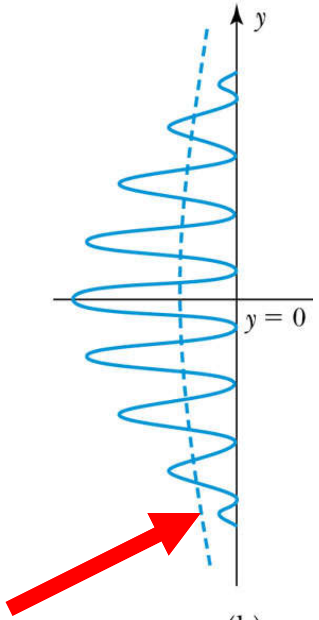
Figure 5-19 A three-dimensional wave packet representing a particle moving along the x axis. The dot indicates the position of a classical particle. Note that the packet spreads out in the x and y directions. This spreading is due to dispersion, resulting from the fact that the phase velocity of the individual waves making up the packet depends on the wavelength of the waves.

5.5: Waves or Particles?

- Young’s double-slit diffraction experiment demonstrates the wave property of light.
- However, dimming the light results in single flashes on the screen representative of particles.



(a)

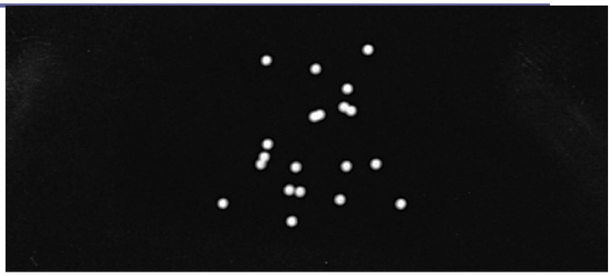


(b)

L>>d,
far field

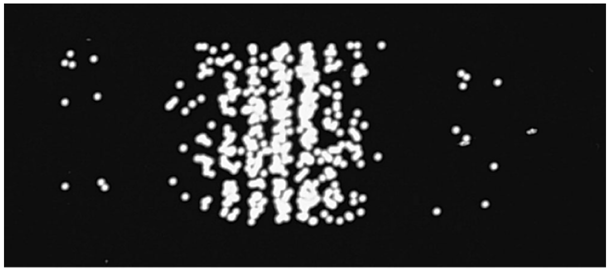
Wrong !

Same applies to particles with mass !!!!

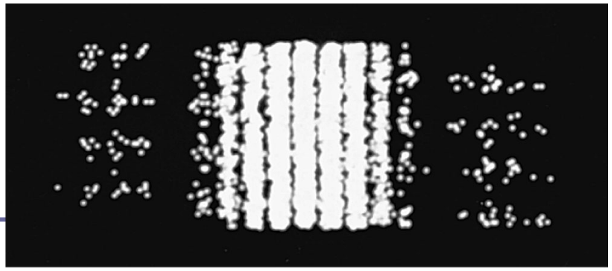


(a) 20 counts

(b) 100 counts



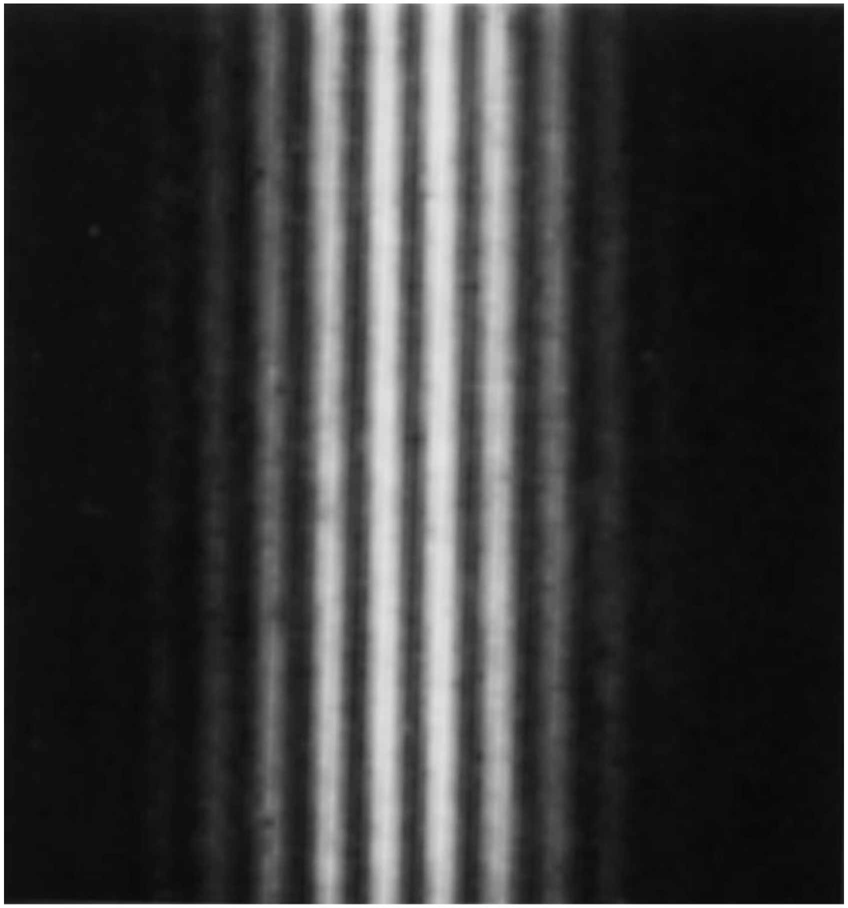
(c) 500 counts

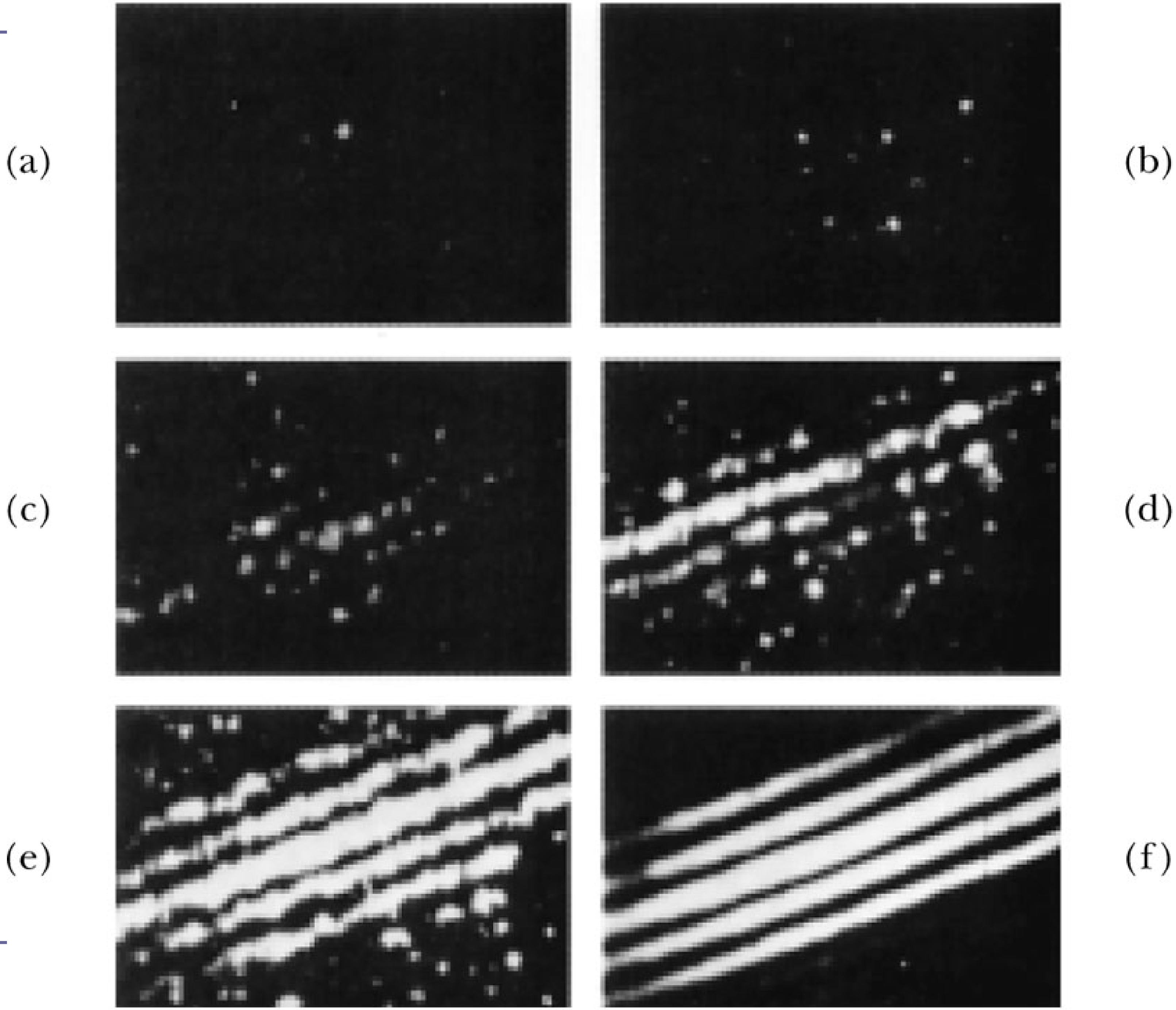


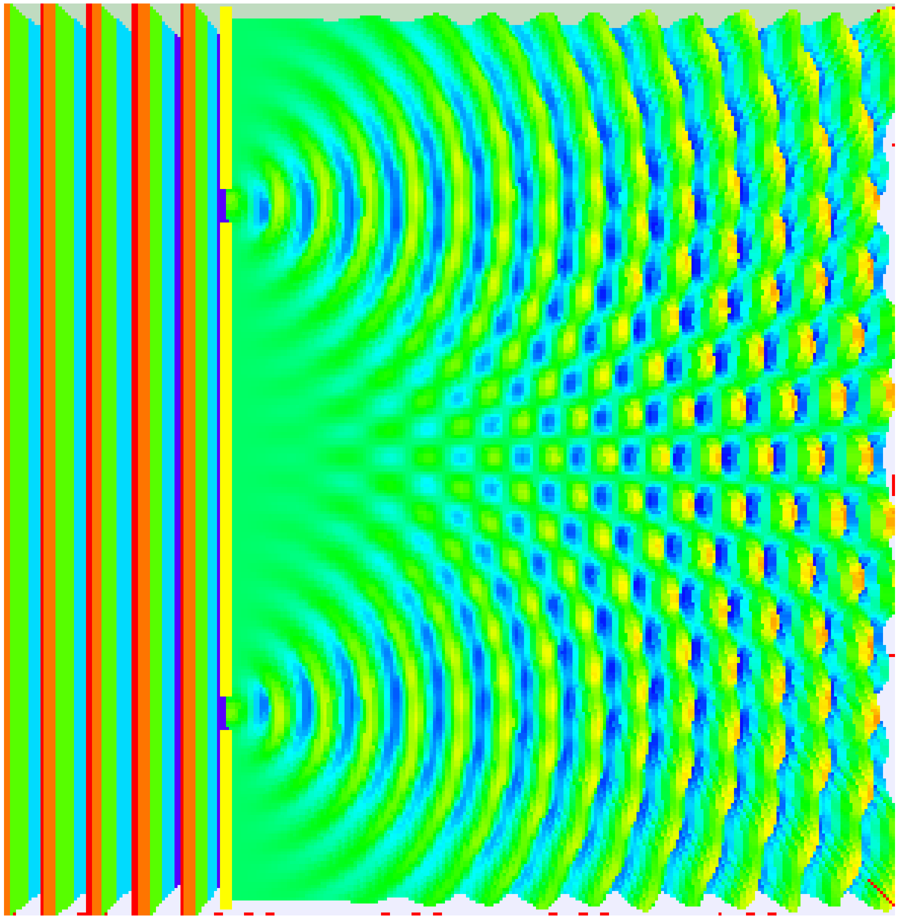
(d) ~4000 counts

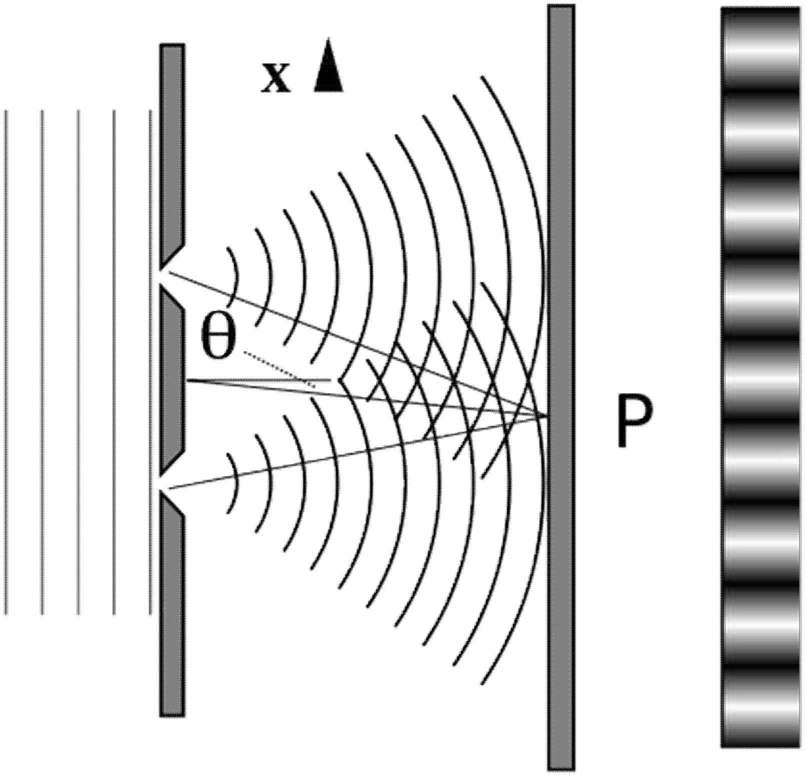
Electron Double-Slit Experiment

- C. Jönsson of Tübingen, Germany, succeeded in 1961 in showing double-slit interference effects for **electrons** by constructing very narrow slits and using relatively large distances between the slits and the observation screen.
- This experiment demonstrated that precisely the same behavior occurs for both light (waves) and electrons (particles).



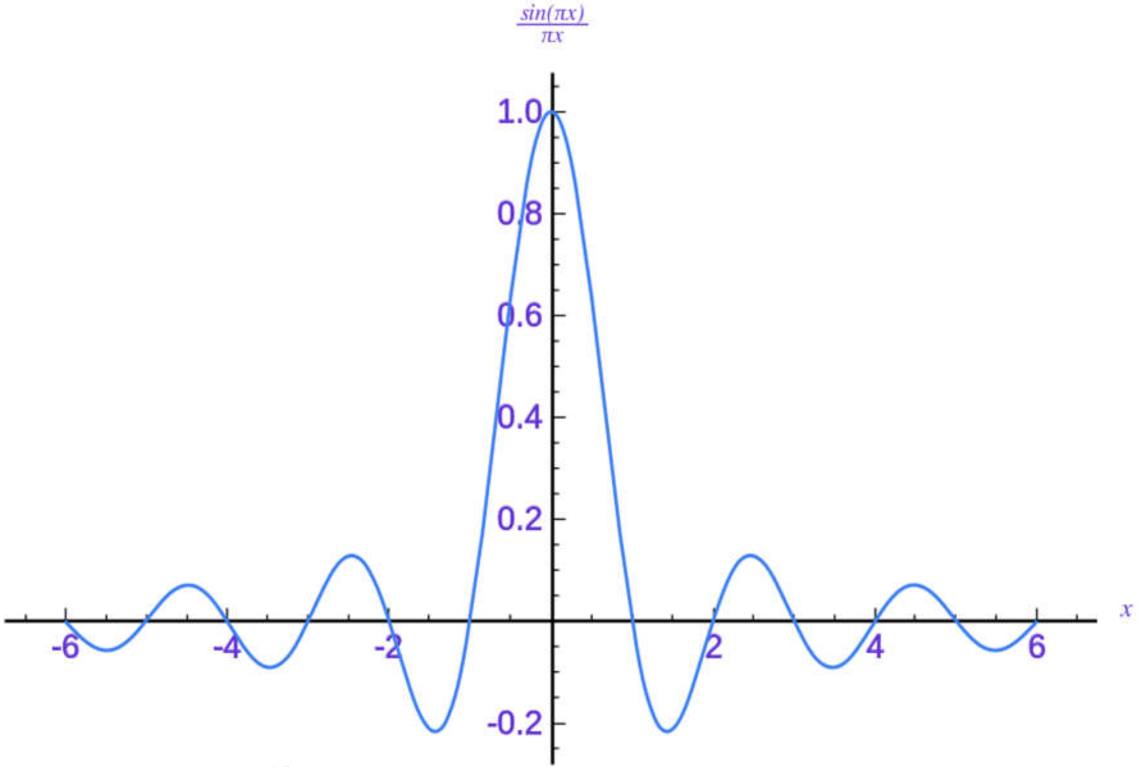

(a)
(b)
(c)
(d)
(e)
(f)

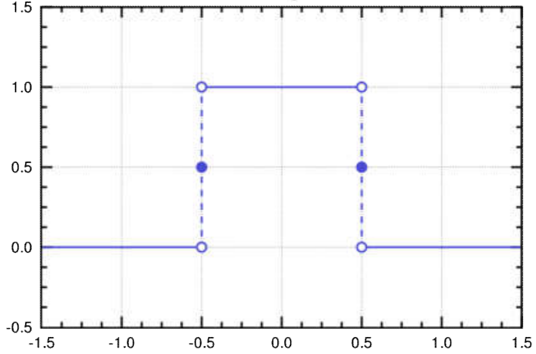




http://en.wikipedia.org/wiki/Double-slit_experiment

sinc function, is the Fourier transform of the rectangular function



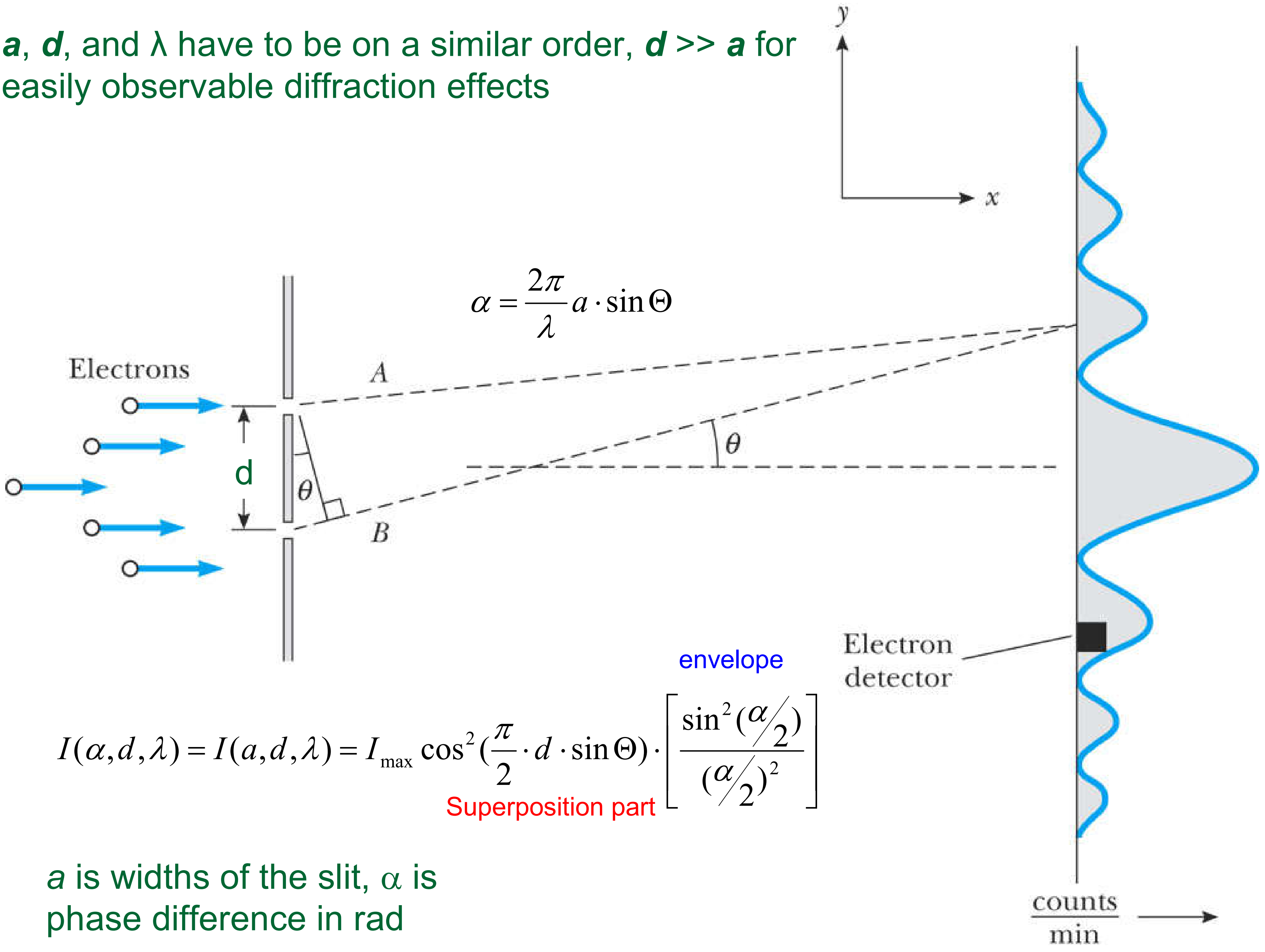


For any wave, the local amplitude squared gives the local intensity, number of constituent particles

Same applies in principle to wave functions

See also: http://en.wikipedia.org/wiki/Sinc_function

a, ***d***, and λ have to be on a similar order, ***d*** >> ***a*** for easily observable diffraction effects



$$\alpha = \frac{2\pi}{\lambda} a \cdot \sin\Theta$$

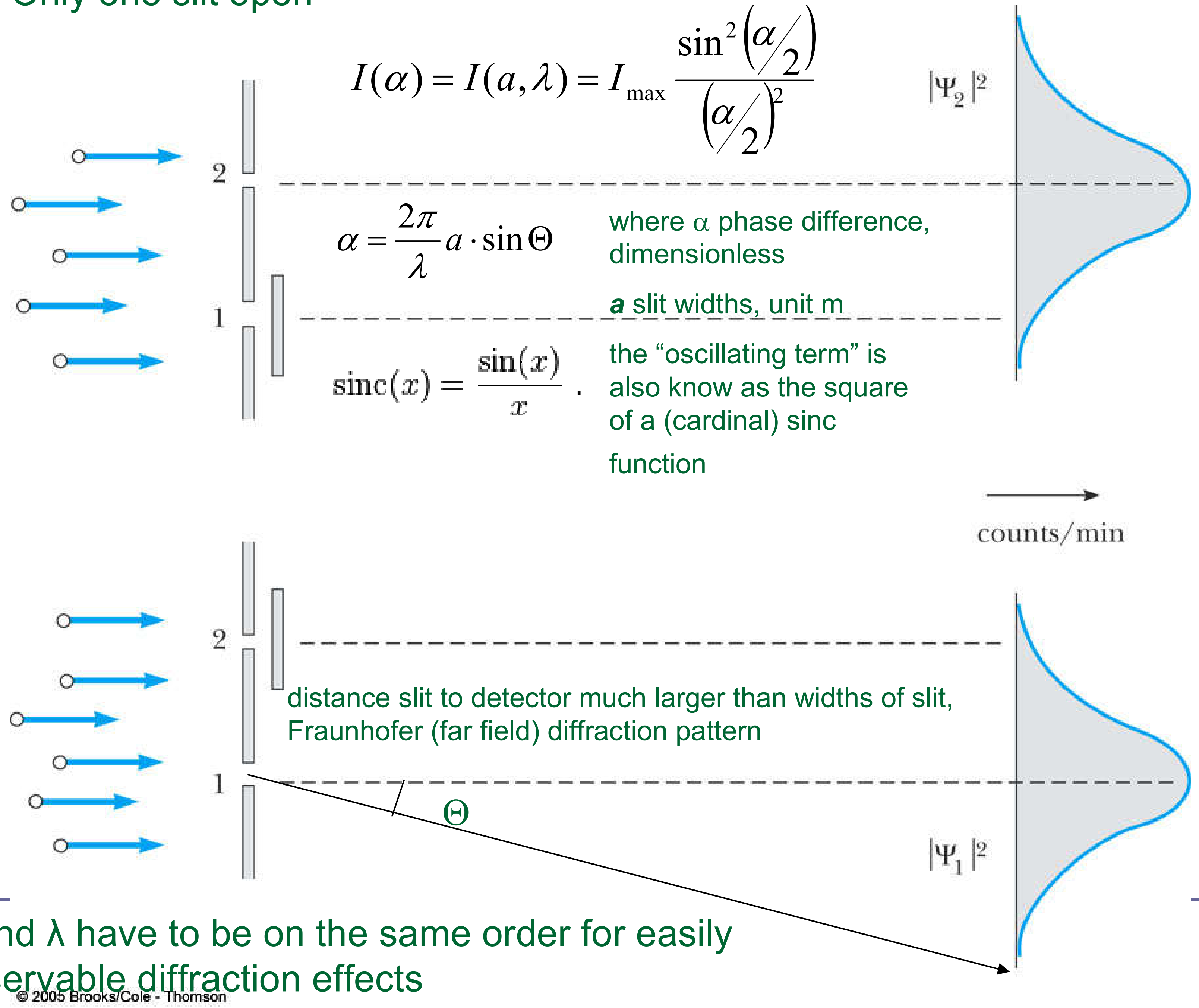
envelope

$$I(\alpha,d,\lambda) = I(a,d,\lambda) = I_{\max} \cos^2(\frac{\pi}{2} \cdot d \cdot \sin\Theta) \cdot \left[\frac{\sin^2(\alpha/2)}{(\alpha/2)^2} \right]$$

Superposition part

a is widths of the slit, α is phase difference in rad

Only one slit open



$$I(\alpha) = I(a,\lambda) = I_{\max}\frac{\sin^2\left(\alpha/2\right)}{\left(\alpha/2\right)^2}$$

$$\alpha = \frac{2\pi}{\lambda}a \cdot \sin\Theta$$

where α phase difference, dimensionless

a slit widths, unit m

$$\mathrm{sinc}(x) = \frac{\sin(x)}{x}\,.$$

the “oscillating term” is also know as the square of a (cardinal) sinc

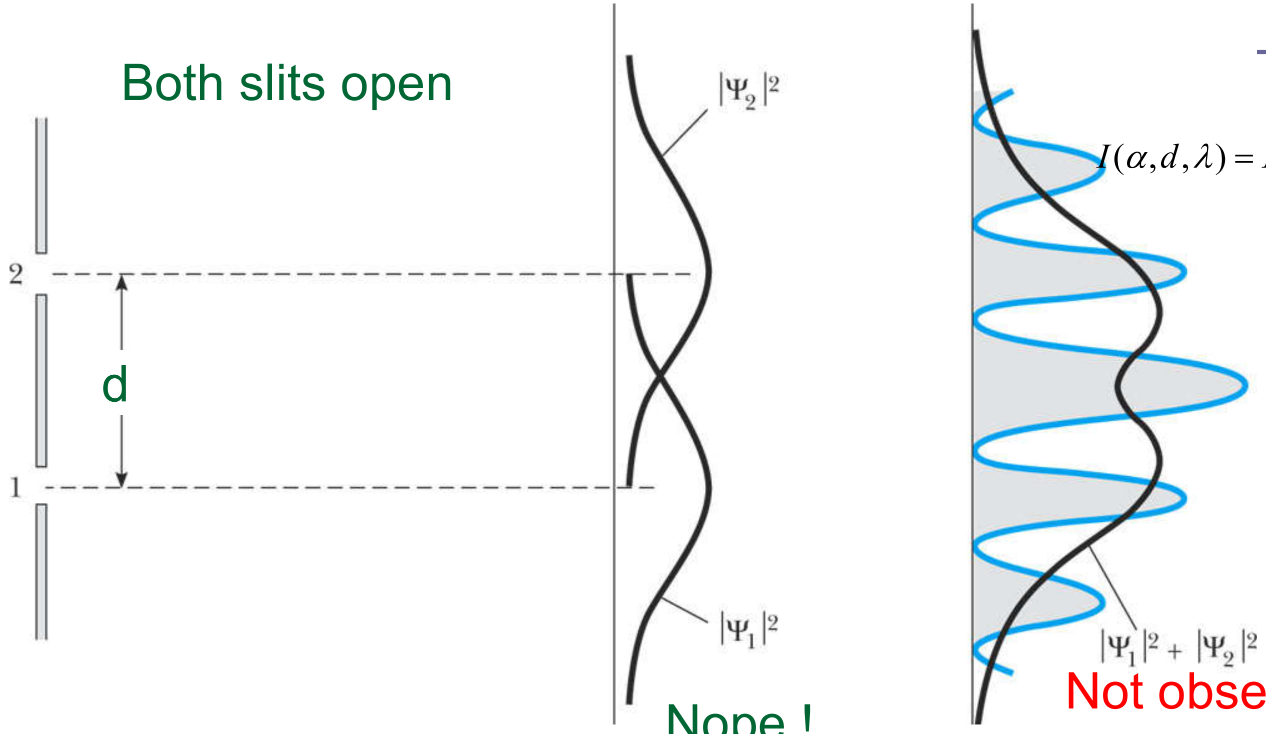
function

distance slit to detector much larger than widths of slit, Fraunhofer (far field) diffraction pattern

a and λ have to be on the same order for easily observable diffraction effects

© 2005 Brooks/Cole - Thomson

Both slits open



$$I(\alpha,d,\lambda) = I(a,d,\lambda) = I_{\max}\cos^2\left(\frac{\pi}{2}\cdot d\cdot\sin\Theta\right)\cdot\left[\frac{\sin^2(\alpha/2)}{(\alpha/2)^2}\right]$$

path difference α and ***a*** (slit widths) as defined earlier for single slit; ***d*** distance between the two slits, for easy observation of diffraction, ***d*** and λ of the same order, also ***d*** >> ***a***

Nope !

Not observed

$$\alpha = \frac{2\pi}{\lambda}a\cdot\sin\Theta$$

Table 5.1

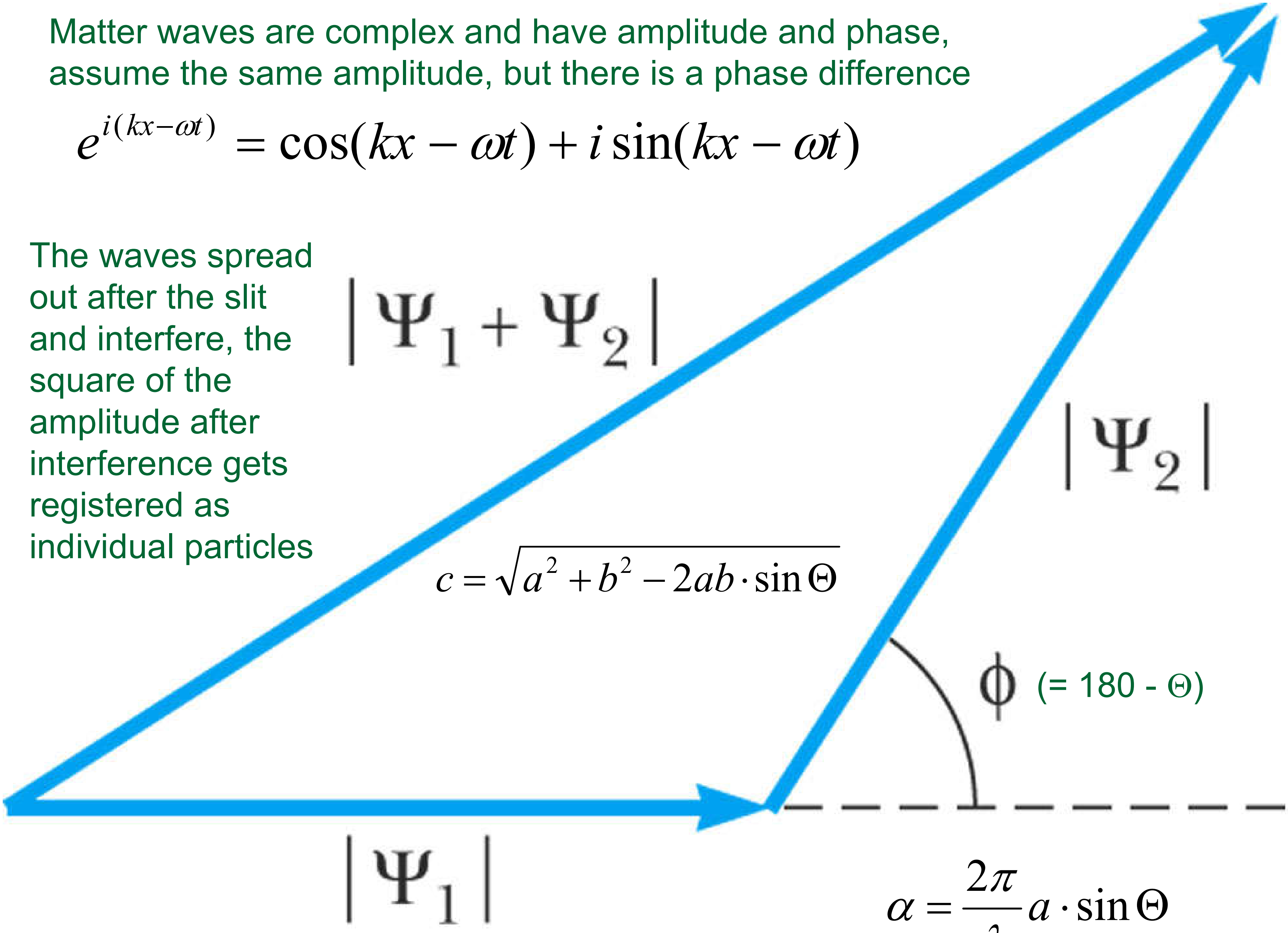
Case	Wavefunction	Counts/Minute at Screen
Electron is measured to pass through slit 1 or slit 2	Ψ_1 or Ψ_2	$\lvert\Psi_1\rvert^2 + \lvert\Psi_2\rvert^2$
No measurements made on electron at slits	$\Psi_1 + \Psi_2$	$\lvert\Psi_1\rvert^2 + \lvert\Psi_2\rvert^2 + 2\lvert\Psi_1\rvert\lvert\Psi_2\rvert\cos\phi$

If you don’t have information on which slit the particle went through, you have the interference pattern, ask Andres La Rosa

Matter waves are complex and have amplitude and phase, assume the same amplitude, but there is a phase difference

$$e^{i(kx-\omega t)} = \cos(kx-\omega t) + i\sin(kx-\omega t)$$

The waves spread out after the slit and interfere, the square of the amplitude after interference gets registered as individual particles



(= 180 - Θ)

$$c = \sqrt{a^2 + b^2 - 2ab \cdot \sin\Theta}$$

$$\alpha = \frac{2\pi}{\lambda} a \cdot \sin\Theta$$

Which slit? – standard explanation

- To determine which slit the **electron** went through: We set up a light shining on the double slit and use a powerful 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 (we gained which-way information).
- Use a subscript “ph” to denote variables for light (photon). Therefore the momentum of the photon is

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

- The momentum of the electrons will be on the order of $p_{\mathrm{el}} = \frac{h}{\lambda_{\mathrm{el}}} \sim \frac{h}{d}$.
- The difficulty is that the momentum of the photons used to determine which slit the electron went through is sufficiently great to strongly modify the momentum of the electron itself, thus changing the direction of the electron! The attempt to identify which slit the electron is passing through will in itself destroy the double slit interference pattern.

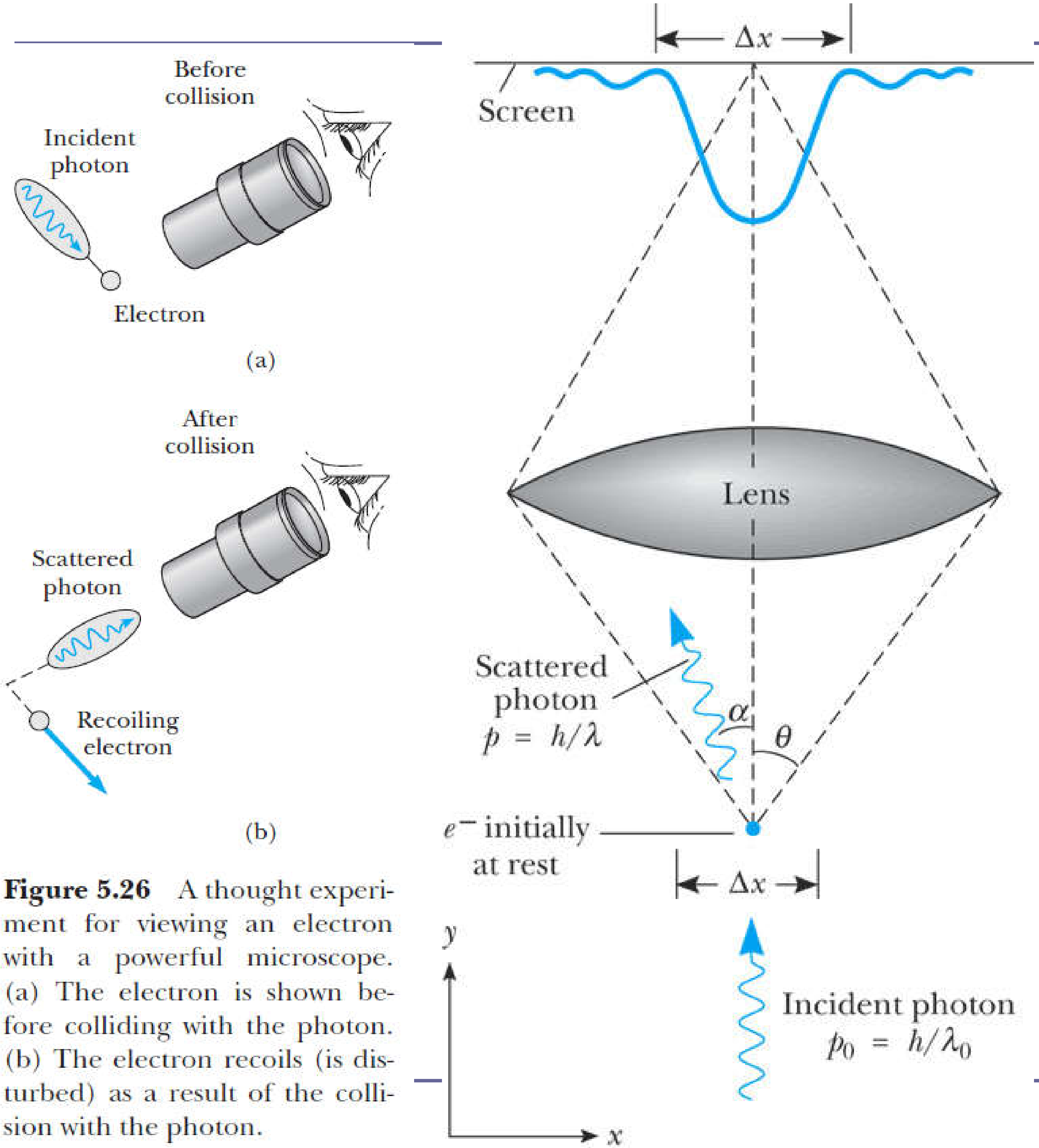
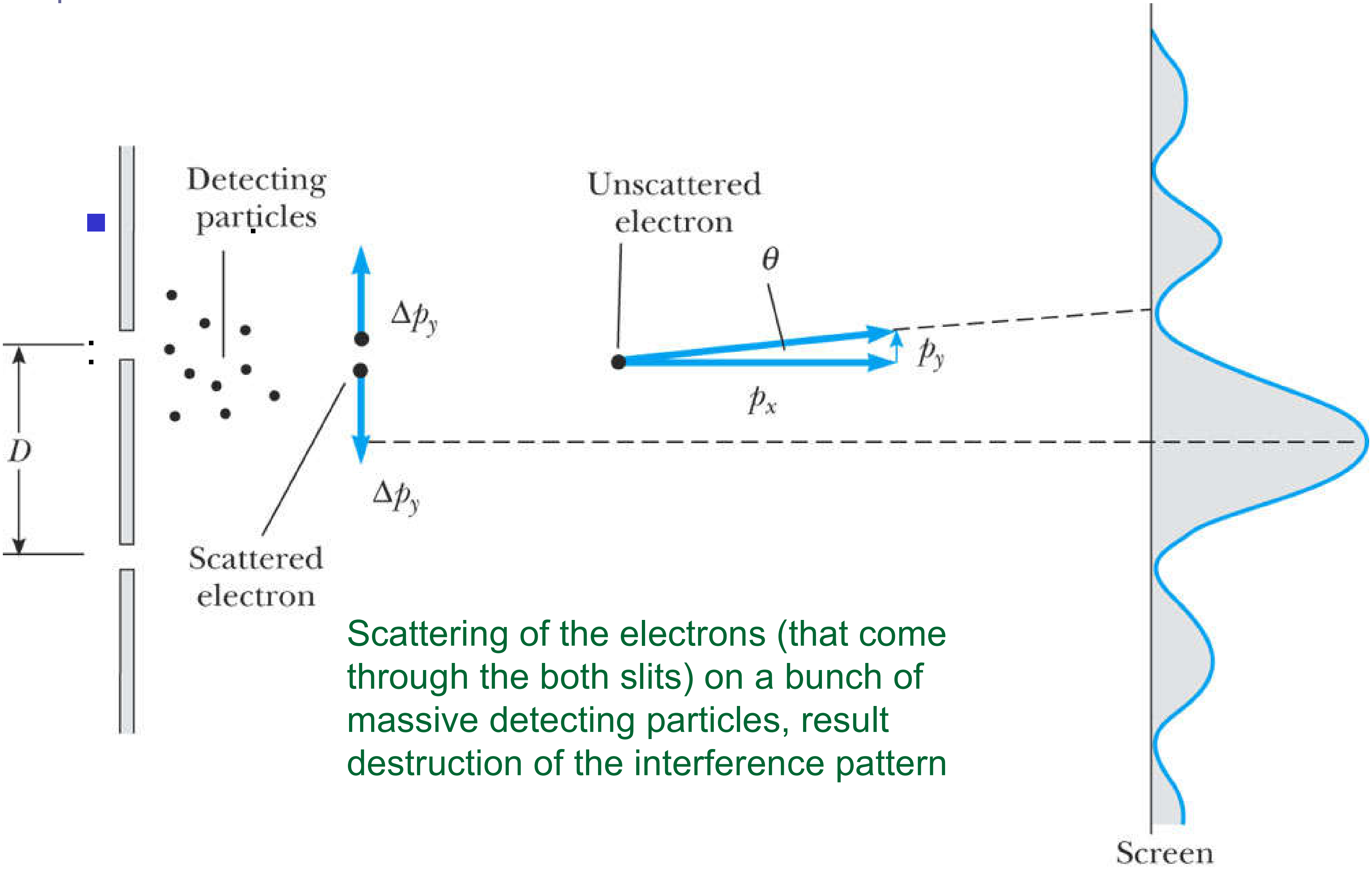


Figure 5.26 A thought experiment for viewing an electron with a powerful microscope. (a) The electron is shown before colliding with the photon. (b) The electron recoils (is disturbed) as a result of the collision with the photon.

Since the uncertainty principle is really a statement about accuracy rather than precision, there is a non-classical kind of “systematic rest error” that cannot be corrected for

In classical physics this is simply ignored as things are large in comparison to electrons, atoms, molecules, nano-crystals …



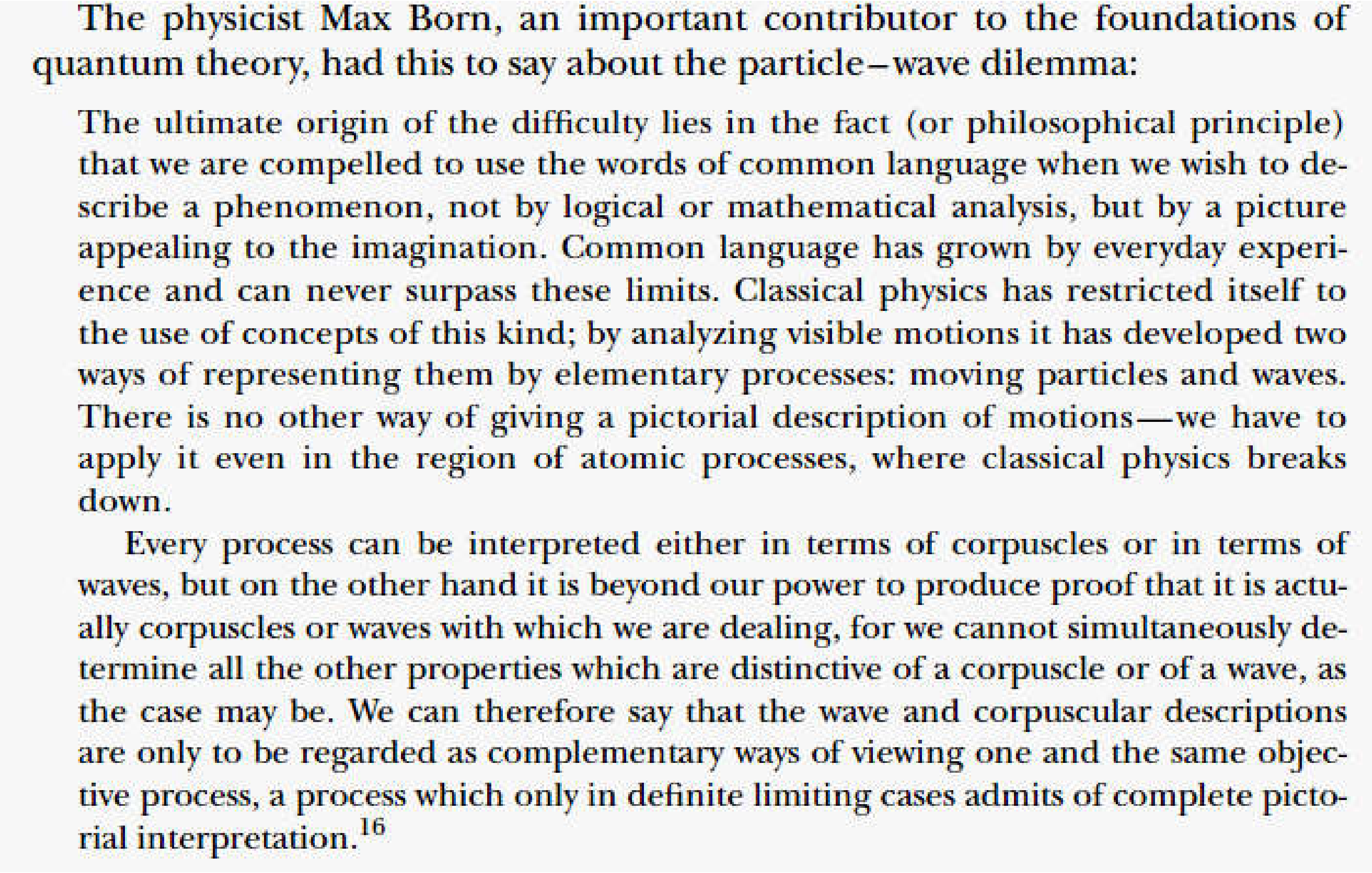
Scattering of the electrons (that come through the both slits) on a bunch of massive detecting particles, result destruction of the interference pattern

For more what is really going on. PH 411 Andres LaRosa

The Copenhagen Interpretation

- Copenhagen's interpretation of the wave function (quantum mechanics in its "final" and current form) consists of **3** (to 4) principles:
  1) **The complementarity principle of Bohr**
  2) **The uncertainty principle of Heisenberg**
  3) **The statistical interpretation of Born, based on detection probabilities determined by squares of wave functions**
  4) Bohr's correspondence principle (for reasonable quantum mechanics ideas) – doesn't capture wave – particle duality, build bridge to classical physics, ad hoc quantization to explain the spectral lines of hydrogen-like atoms and +ions

- Together these concepts form a logical interpretation of the physical meaning of quantum theory. According to the Copenhagen interpretation, physics needs to make predictions on the outcomes of future experiments (measurement) on the basis of the theoretical analysis of previous experiments (measurements)
- Physics is not about "***the truth***", questions that cannot be answered by experiments (measurements) are meaningless to the modern physicist. Philosophers, priests, gurus, … can be asked these questions and often answer them. Problem: they tend to disagree … (and want to get paid)



The physicist Max Born, an important contributor to the foundations of quantum theory, had this to say about the particle–wave dilemma:

> The ultimate origin of the difficulty lies in the fact (or philosophical principle) that we are compelled to use the words of common language when we wish to describe a phenomenon, not by logical or mathematical analysis, but by a picture appealing to the imagination. Common language has grown by everyday experience and can never surpass these limits. Classical physics has restricted itself to the use of concepts of this kind; by analyzing visible motions it has developed two ways of representing them by elementary processes: moving particles and waves. There is no other way of giving a pictorial description of motions—we have to apply it even in the region of atomic processes, where classical physics breaks down.
>
> Every process can be interpreted either in terms of corpuscles or in terms of waves, but on the other hand it is beyond our power to produce proof that it is actually corpuscles or waves with which we are dealing, for we cannot simultaneously determine all the other properties which are distinctive of a corpuscle or of a wave, as the case may be. We can therefore say that the wave and corpuscular descriptions are only to be regarded as complementary ways of viewing one and the same objective process, a process which only in definite limiting cases admits of complete pictorial interpretation.[16]

5.8: Particle in an infinitely deep Box

- A particle of mass *m* is trapped in a one-dimensional box of width *l*, ***but not under the influence of a force, so no potential energy***
- The particle is treated as a standing wave.
- The box puts boundary conditions on the wave. The wave function must be zero at the walls of the box and on the outside.
- In order for the probability to vanish at the walls, we must have an integral number of half wavelengths in the box.

$$\frac{n\lambda}{2} = \ell \quad \text{or} \quad \lambda_n = \frac{2\ell}{n} \quad (n = 1, 2, 3, \ldots) \qquad p = \hbar k = h/\lambda$$

- The energy of the particle is

$$E = \text{K.E.} = \frac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2}$$

- As wavelengths and momenta are quantized, so will be total energy (which is all kinetic (as potential energy inside box is zero, infinity outside)

$$E_n = \frac{h^2}{2m}\left(\frac{n}{2\ell}\right)^2 = n^2\frac{h^2}{8m\ell^2} \quad (n = 1, 2, 3, \ldots)$$

- A particle in a box will possess at any one time one of these discrete energies. Transitions between the energy levels are possible, if the particle is charged, these transitions are akin to the spectral lines of atoms.

Probability of finding the Particle in a certain region of space

- The probability of observing the particle between *x* and *x* + *dx* in each state is

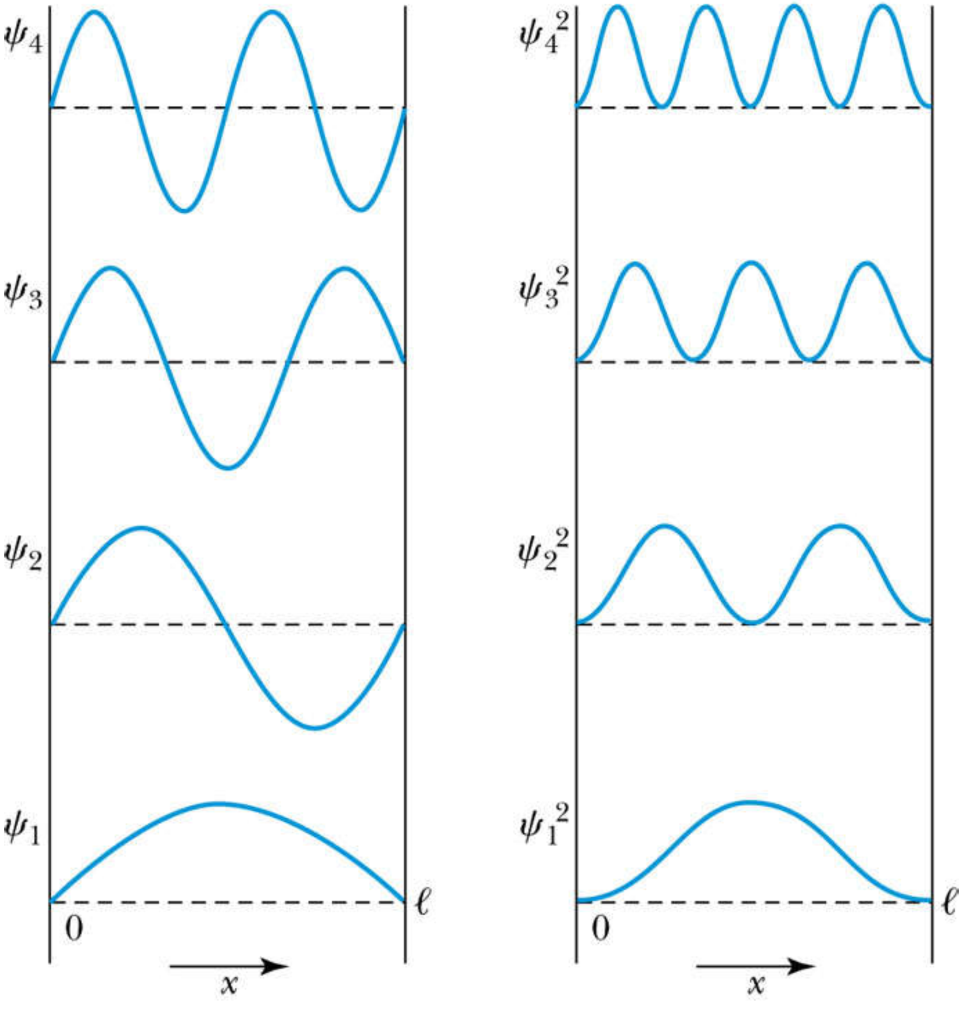
$$P_n\,dx \propto \left|\Psi_n(x)\right|^2 dx$$

Since there is dx, we need to integrate over the region we are interested in

All other observable quantities will be obtained by integrations as well.

- Note that $E_0 = 0$ is not a possible energy level, there is no quantum number n = 0, so E_1 is ground state also called zero point energy in a quantum oscillator

- The concept of energy levels, as first discussed in the Bohr model, has surfaced in a natural way by using matter waves.



We analyze the same model in the next chapter with operators on wave functions and expectation value integrals (that tell us all there can be known)

Minimum Energy of a Particle in a Box

$$\Delta p_x \cdot \Delta x \approx \hbar$$

An important consequence of the uncertainty principle is that a particle confined to a finite space cannot have zero kinetic energy. Let us consider the case of a one-dimensional "box" of length L. If we know that the particle is in the box, Δx is not larger than L. This implies that Δp is at least $\hbar/L$. (Since we are interested in orders of magnitude, we will ignore the 1/2 in the minimum uncertainty product. In general, distributions are not Gaussian anyway, so $\Delta p \Delta x$ will be larger than $\hbar/2$.) Let us take the standard deviation as a measure of Δp,

$$(\Delta p)^2 = (p - \overline{p})^2_{\text{av}} = (p^2 - 2p\overline{p} + \overline{p}^2)_{\text{av}} = \overline{p^2} - \overline{p}^2$$

If the box is symmetric, $\overline{p}$ will be zero since the particle moves to the left as often as to the right. Then

$$(\Delta p)^2 = \overline{p^2} \geq \left(\frac{\hbar}{L}\right)^2$$

This formula was derived earlier, n = 1

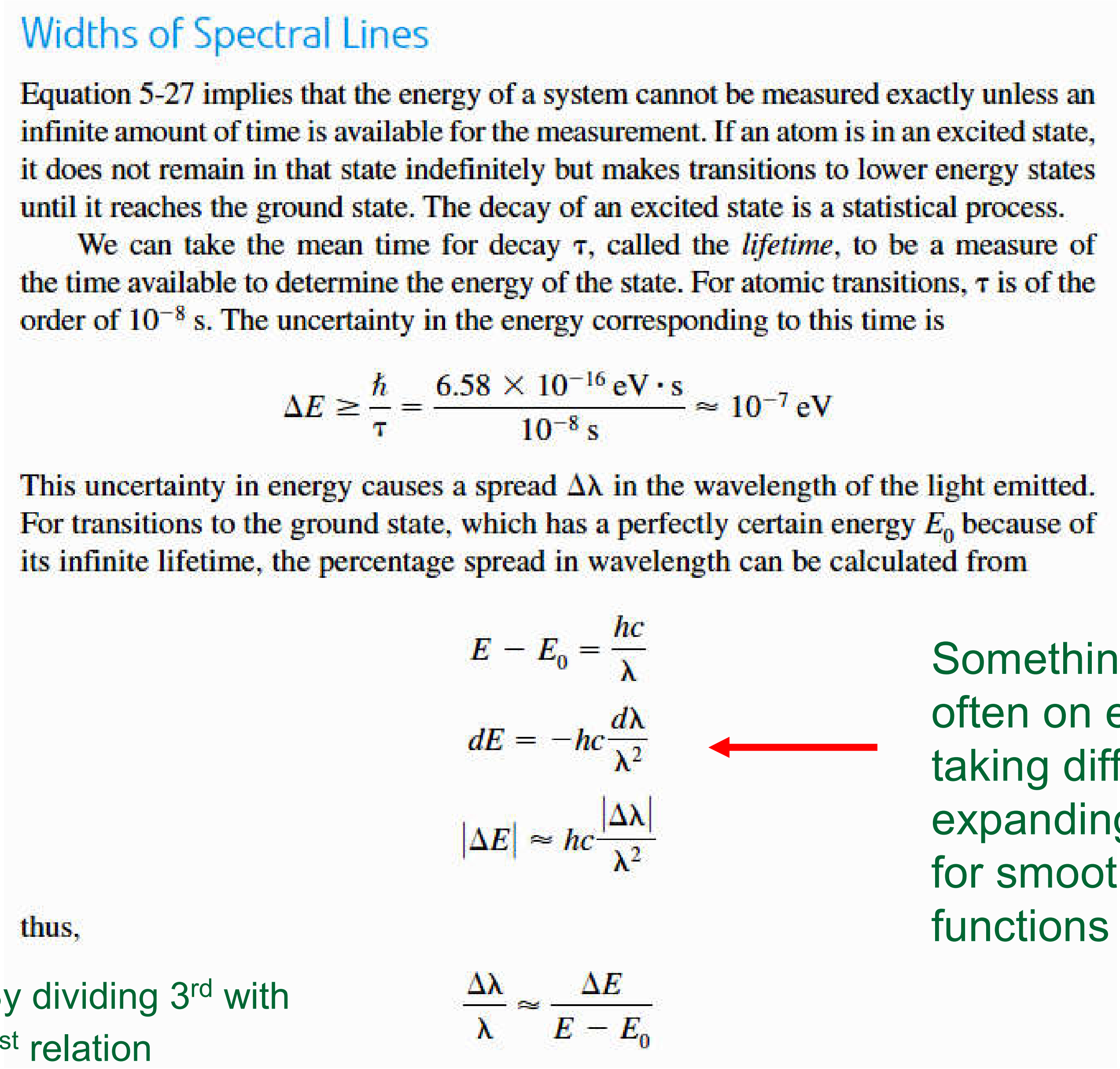
$$E_n = \frac{h^2}{2m}\left(\frac{n}{2\ell}\right)^2 = n^2\frac{h^2}{8m\ell^2} \qquad (n = 1, 2, 3, \ldots)$$

and the average kinetic energy is

$$\overline{E} = \frac{\overline{p^2}}{2m} \geq \frac{\hbar^2}{2mL^2} \qquad \textbf{5-28}$$

Pretty good match for low n

Thus, we see that the uncertainty principle indicates that the minimum energy of a particle (*any* particle) in a "box" (*any* kind of "box") cannot be zero. This minimum energy given by Equation 5-28 for a particle in a one-dimensional box is called the *zero point energy*.



Widths of Spectral Lines

Equation 5-27 implies that the energy of a system cannot be measured exactly unless an infinite amount of time is available for the measurement. If an atom is in an excited state, it does not remain in that state indefinitely but makes transitions to lower energy states until it reaches the ground state. The decay of an excited state is a statistical process.

We can take the mean time for decay τ, called the *lifetime*, to be a measure of the time available to determine the energy of the state. For atomic transitions, τ is of the order of 10^{-8} s. The uncertainty in the energy corresponding to this time is

$$\Delta E \geq \frac{\hbar}{\tau} = \frac{6.58 \times 10^{-16}\ \mathrm{eV \cdot s}}{10^{-8}\ \mathrm{s}} \approx 10^{-7}\ \mathrm{eV}$$

This uncertainty in energy causes a spread $\Delta\lambda$ in the wavelength of the light emitted. For transitions to the ground state, which has a perfectly certain energy E_0 because of its infinite lifetime, the percentage spread in wavelength can be calculated from

$$E - E_0 = \frac{hc}{\lambda}$$

$$dE = -hc\frac{d\lambda}{\lambda^2}$$

$$|\Delta E| \approx hc\frac{|\Delta\lambda|}{\lambda^2}$$

thus,

$$\frac{\Delta\lambda}{\lambda} \approx \frac{\Delta E}{E - E_0}$$

$$\Delta E \cdot \Delta t \approx \hbar$$

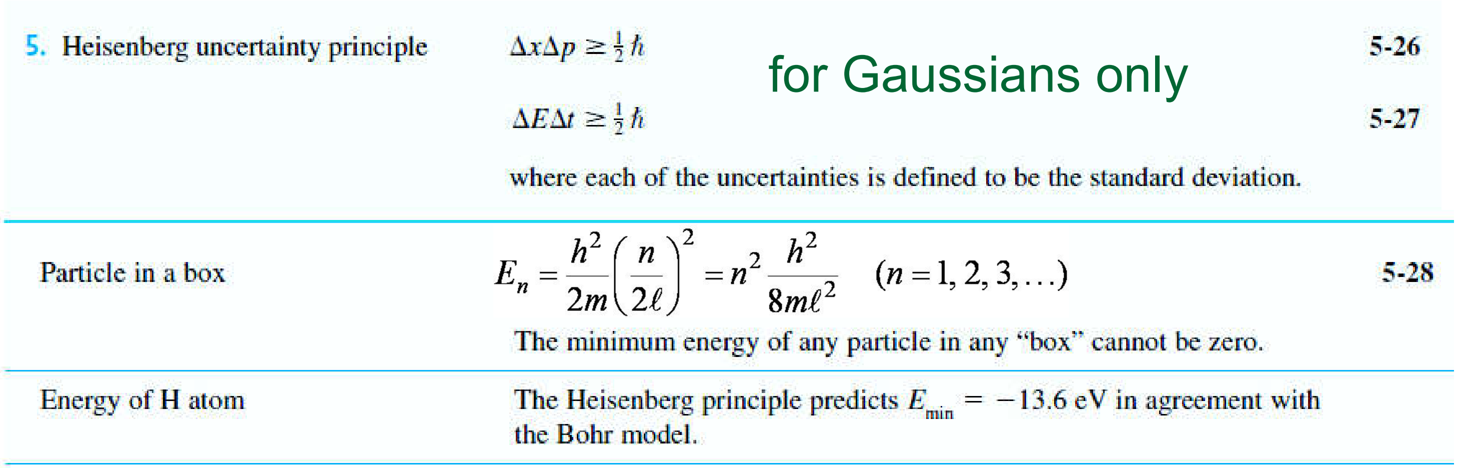
Something like that is often on exams, i.e. first taking differentials, then expanding into deltas for smoothly varying functions

By dividing 3rd with 1st relation

The energy width $\Delta E = \hbar/\tau$ is called the *natural line width*

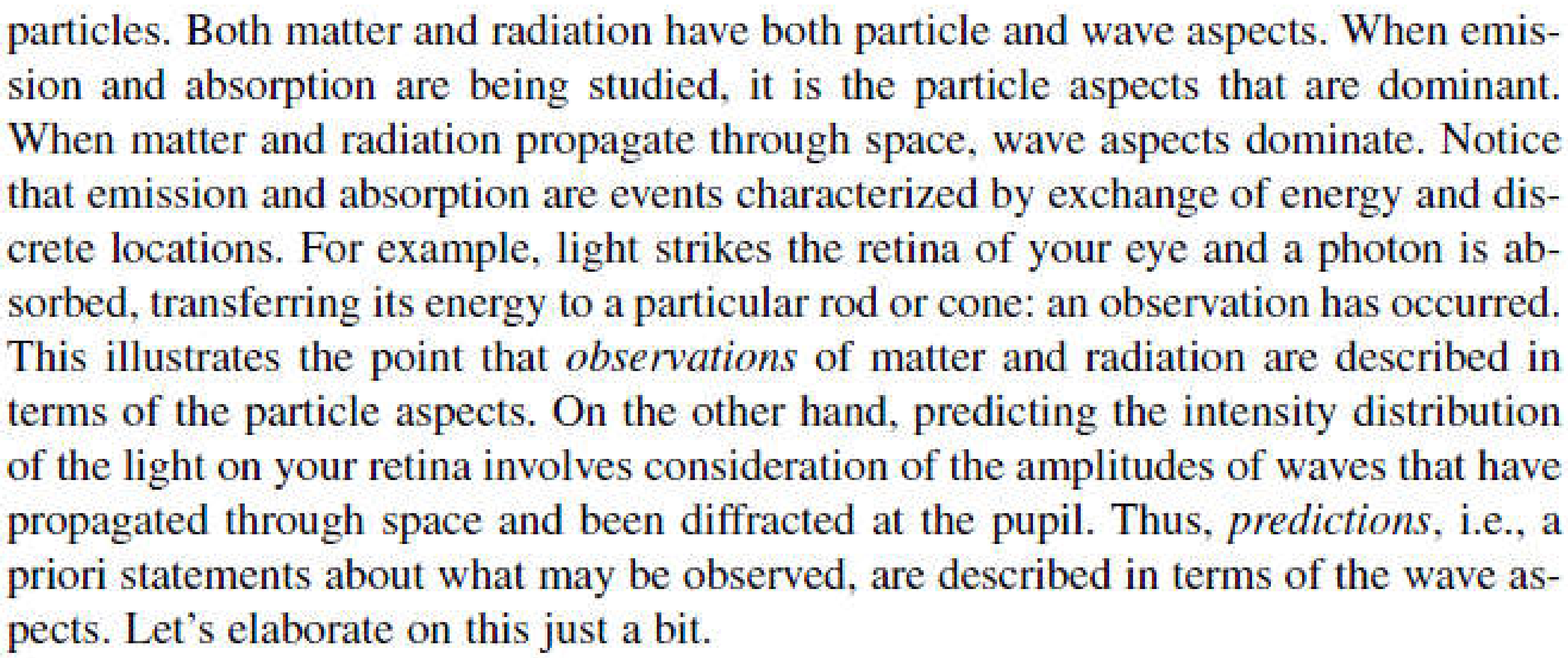
TOPIC	RELEVANT EQUATIONS AND REMARKS	
1. De Broglie relations	$f = E/h$	5-1
	$\lambda = h/p$	5-2
	Electrons and all other particles exhibit the wave properties of interference and diffraction	
2. Detecting electron waves		
Davisson and Germer	Showed that electron waves diffracted from a single Ni crystal according to Bragg's equation	
	$n\lambda = D \sin\varphi$	5-5
3. Wave packets		
Wave equation	$\frac{d^2y}{dx^2} = \frac{1}{v^2}\frac{d^2y}{dt^2}$	5-11
Uncertainty relations	$\Delta k \Delta x \sim 1$	5-17
	$\Delta\omega\Delta t \sim 1$	5-18
Wave speed	$v_p = f\lambda = \omega/k$	
Group (packet) speed	$v_g = \frac{d\omega}{dk} = v_p + k\frac{dv_p}{dk}$	5-16
Matter waves	The wave packet moves with the particle speed; i.e., the particle speed is the group speed v_g.	
4. Probabilistic interpretation	The magnitude square of the wave function is proportional to the probability of observing a particle in the region dx at x and t.	
	$P(x)dx = \lvert\Psi\rvert^2 dx$	5-23

Much better to only use Bragg's equation and remember that between primary beam and diffraction beam there is always 2Θ



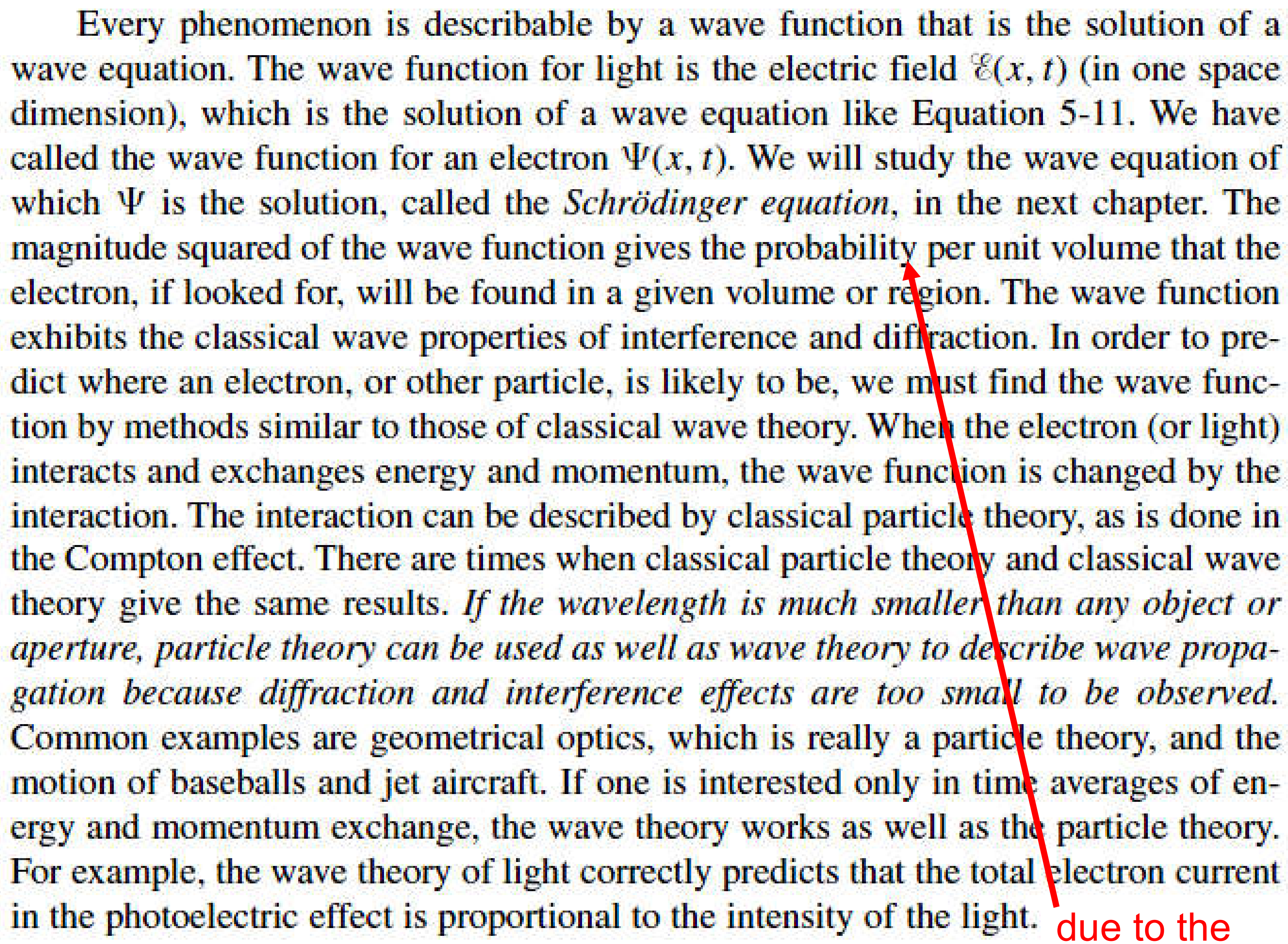
5. Heisenberg uncertainty principle	$\Delta x \Delta p \geq \frac{1}{2}\hbar$	5-26
	$\Delta E \Delta t \geq \frac{1}{2}\hbar$	5-27
	where each of the uncertainties is defined to be the standard deviation.	
Particle in a box	$E_n = \frac{h^2}{2m}\left(\frac{n}{2\ell}\right)^2 = n^2\frac{h^2}{8m\ell^2} \quad (n = 1, 2, 3, \ldots)$ The minimum energy of any particle in any "box" cannot be zero.	5-28
Energy of H atom	The Heisenberg principle predicts $E_{\text{min}} = -13.6$ eV in agreement with the Bohr model.	

for Gaussians only



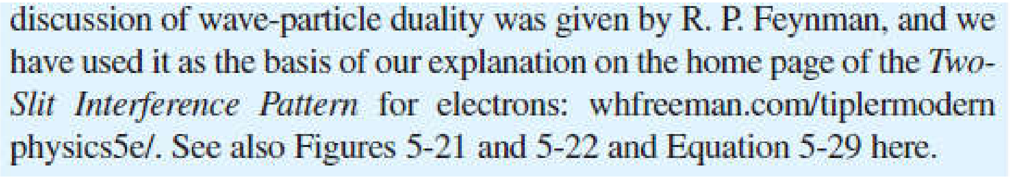
particles. Both matter and radiation have both particle and wave aspects. When emission and absorption are being studied, it is the particle aspects that are dominant. When matter and radiation propagate through space, wave aspects dominate. Notice that emission and absorption are events characterized by exchange of energy and discrete locations. For example, light strikes the retina of your eye and a photon is absorbed, transferring its energy to a particular rod or cone: an observation has occurred. This illustrates the point that *observations* of matter and radiation are described in terms of the particle aspects. On the other hand, predicting the intensity distribution of the light on your retina involves consideration of the amplitudes of waves that have propagated through space and been diffracted at the pupil. Thus, *predictions*, i.e., a priori statements about what may be observed, are described in terms of the wave aspects. Let's elaborate on this just a bit.

$$e^{i(kx-\omega t)} = \cos(kx - \omega t) + i\sin(kx - \omega t)$$



Every phenomenon is describable by a wave function that is the solution of a wave equation. The wave function for light is the electric field $\mathscr{E}(x, t)$ (in one space dimension), which is the solution of a wave equation like Equation 5-11. We have called the wave function for an electron $\Psi(x, t)$. We will study the wave equation of which Ψ is the solution, called the *Schrödinger equation*, in the next chapter. The magnitude squared of the wave function gives the probability per unit volume that the electron, if looked for, will be found in a given volume or region. The wave function exhibits the classical wave properties of interference and diffraction. In order to predict where an electron, or other particle, is likely to be, we must find the wave function by methods similar to those of classical wave theory. When the electron (or light) interacts and exchanges energy and momentum, the wave function is changed by the interaction. The interaction can be described by classical particle theory, as is done in the Compton effect. There are times when classical particle theory and classical wave theory give the same results. *If the wavelength is much smaller than any object or aperture, particle theory can be used as well as wave theory to describe wave propagation because diffraction and interference effects are too small to be observed.* Common examples are geometrical optics, which is really a particle theory, and the motion of baseballs and jet aircraft. If one is interested only in time averages of energy and momentum exchange, the wave theory works as well as the particle theory. For example, the wave theory of light correctly predicts that the total electron current in the photoelectric effect is proportional to the intensity of the light.

due to the uncertainty principle, we can only make statistical inferences



discussion of wave-particle duality was given by R. P. Feynman, and we have used it as the basis of our explanation on the home page of the *Two-Slit Interference Pattern* for electrons: whfreeman.com/tiplermodernphysics5e/. See also Figures 5-21 and 5-22 and Equation 5-29 here.

Position-momentum Uncertainty, summary

- It is impossible to know simultaneously with arbitrary accuracy/precision, the values of *k, p* and *x* for a particle in a bound system. The wave number *k* may be rewritten as

$$k = \frac{2\pi}{\lambda} = \frac{2\pi}{h/p} = p\frac{2\pi}{h} = \frac{p}{\hbar}$$

- For the case of a Gaussian wave packet we have

$$\Delta k\,\Delta x = \frac{\Delta p}{\hbar}\Delta x = \frac{1}{2}$$

for a Gaussian wave packet being a very particular case of "minimal extend in space and time" , we have as Heisenberg's **uncertainty principle**:

$$\Delta p_x\,\Delta x \geq \frac{\hbar}{2}$$

A free particle has the very same probability density per unit length and time everywhere, so it can be found "everywhere/anywhere with the same very low probability", but it can have any value of momentum and kinetic energy as it is not part of a bound system

Energy - time Uncertainty summary

- Because we are uncertain of the exact position of a particle, for example an electron somewhere inside an atom (bound by potential energy), the particle can’t have zero kinetic and total energy
- A completely free particle being represented by a complex harmonic wave has no energy uncertainty
- The energy uncertainty of a Gaussian wave packet is

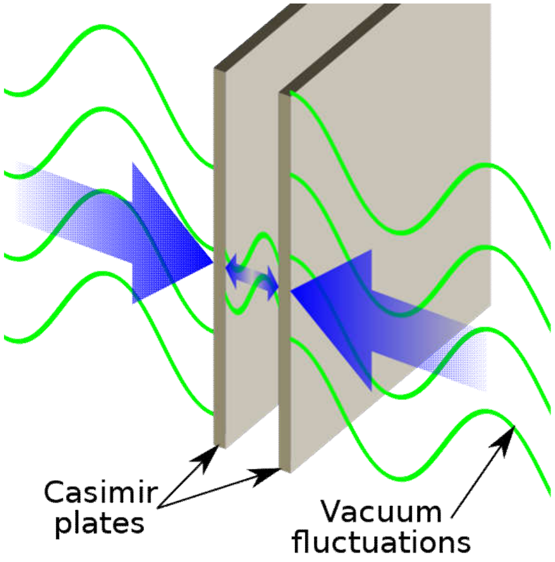
$$\Delta E = h\,\Delta f = h\frac{\Delta\omega}{2\pi} = \hbar\,\Delta\omega \qquad \Delta\omega\,\Delta t = \frac{\Delta E}{\hbar}\Delta t = \frac{1}{2}$$

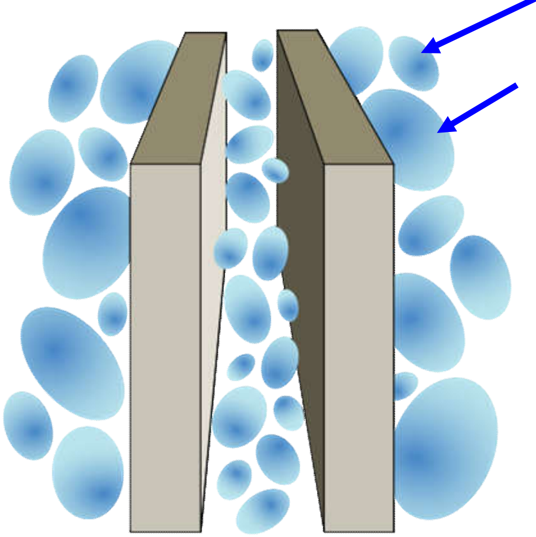
combined with the angular frequency relation

Energy-Time Uncertainty Principle: $\Delta E\,\Delta t \geq \frac{\hbar}{2}$

A bound particle (in a system must have quantized energy levels, with an energy uncertainty that depends on the life time of the particle in anyone state, similarly its kinetic energy and momentum are only knowable within the limits of the uncertainty principle … undisturbed ground state has no ΔE, but still Δp as there is an uncertainty in location

How does a particle ever jump from one energy level to another, it’s again the energy time uncertainty, all fields fluctuate statistically, the electric field being due to virtual photon (we cannot see them because the exist below the uncertainty principle limit) means that virtual photons of different sizes come into being out of “nothing” and disappear into “nothing”





All allowed by the uncertainty principle, we never observe them, but they are there because we have measurable consequences of them in quantum electrodynamics (QED which has been tested to 1 part in 10^{12}), e.g. ***e*** as we know it is the fully screened charge of the electron, at distances smaller than Compton wavelength of an electron charge (***e***) and ***α*** increase

http://en.wikipedia.org/wiki/Casimir_effect

“Because the strength of the force falls off rapidly with distance, it is measurable only when the distance between the objects is extremely small. On a submicron scale, this force becomes so strong that it becomes the dominant force between uncharged conductors. In fact, at separations of 10 nm—about 100 times the typical size of an atom—the Casimir effect produces the equivalent of 1 atmosphere of pressure (101.325 kPa, 1.01325 bar), the precise value depending on surface geometry and other factors.”

better modern physics books such as Beiser mention this