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PHYSICAL PRINCIPLES FOR QUANTUM HARDWARE MODELS

Quantum Mechanics: Short Overview

Emergence of quantum physics

- Blackbody radiation
- Photoelectric effect
- Compton effect
- Bohr atom
- de Broglie and matter waves
- Heisenberg picture and uncertainty relations
- Stern-Gerlach experiment
- The wave function and Schrodinger equation

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Emergence of quantum physics

1. Blackbody radiation

The study of the radiation emmited by a heated body in equilibrium is considered since the XIX century (Kirchoff (1859), Wien (1894))

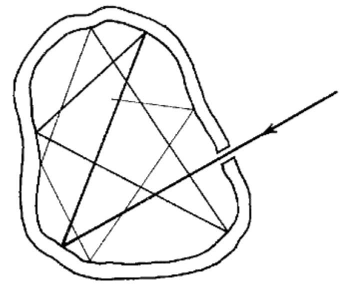

Figure 1-2 A cavity in a body connected by a small hole to the outside. Radiation incident on the hole is completely absorbed after successive reflections on the inner surface of the cavity. The hole absorbs like a blackbody. In the reverse process, in which radiation leaving the hole is built up of contributions emitted from the inner surface, the hole emits like a blackbody.

Experimental results showed that the radiation emitted from a cavity (black body) was related to the energy density of the radiation inside the cavity, as well to the temperature

All figures present in this lecture, unless otherwise noted, are from the book:
QUANTUM PHYSICS of Atoms, Molecules, Solids, Nuclei, and Particles
By Eisberg, Resnick

Emergence of quantum physics

1. Blackbody radiation

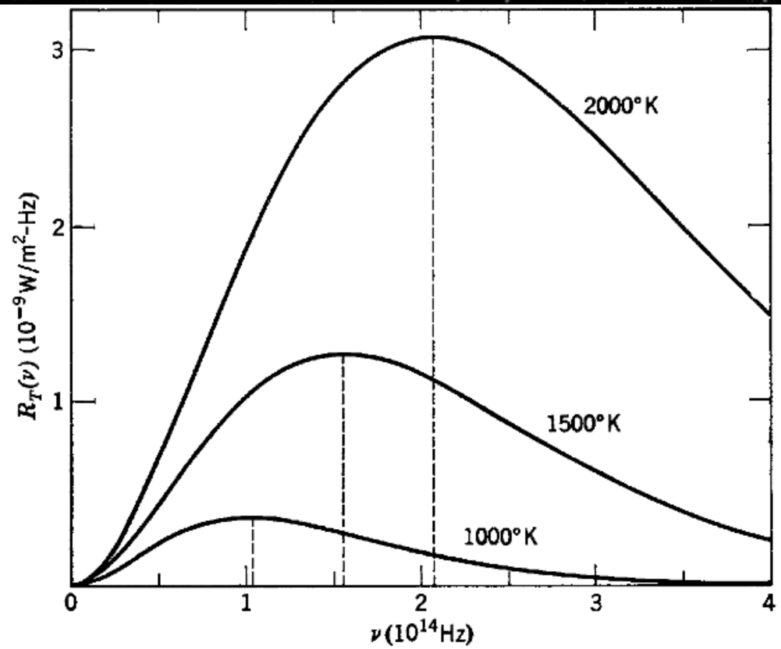

Figure 1-1 The spectral radiancy of a blackbody radiator as a function of the frequency of radiation, shown for temperatures of the radiator of 1000°K, 1500°K, and 2000°K. Note that the frequency at which the maximum radiancy occurs (dashed line) increases linearly with increasing temperature, and that the total power emitted per square meter of the radiator (area under curve) increases very rapidly with temperature.

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1. Blackbody radiation

Rayleigh(1900) , predicted the following result, using the classical theory of radiation in a cavity

$$\rho(v, T) = \frac{8\pi v^2}{c^3} K_B T$$

This result is true only to small frequencies, since the total energy per unit volume (obtained by the integration over all frequencies) is infinity!

Emergence of quantum physics

1. Blackbody radiation

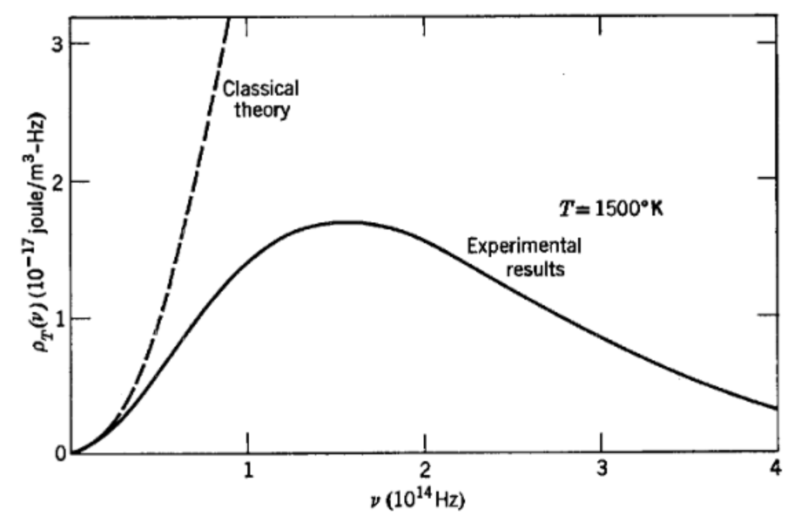

Figure 1-8 The Rayleigh-Jeans prediction (dashed line) compared with the experimental results (solid line) for the energy density of a blackbody cavity, showing the serious discrepancy called the ultraviolet catastrophe.

At the end of 1900, Planck obtained a formula for $\rho(v, T)$ that reads

$$\rho(v, T) = \frac{8\pi h}{c^3} \frac{v^3}{e^{hv/K_B T} - 1}$$

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1. Blackbody radiation

- Planck obtained this formula considering the dynamical equilibrium between the emission and absorption of radiation by the cavity

- Only making the assumption that the radiation of a given frequency *v* could only be emitted or absorbed in quanta of energy E =nh*v*

- $h = 6.625 \times 10^{-34}$ J.s, n = 0, 1, 2, ...

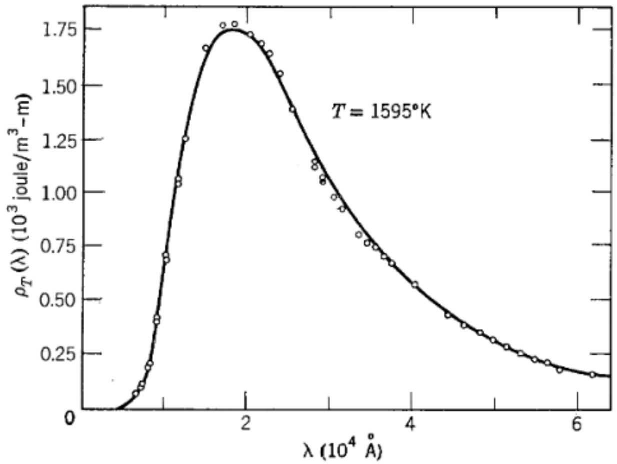

Figure 1-11 Planck's energy density prediction (solid line) compared to the experimental results (circles) for the energy density of a blackbody. The data were reported by Coblentz in 1916 and apply to a temperature of 1595°K. The author remarked in his paper that after drawing the spectral energy curves resulting from his measurements, "owing to eye fatigue it was impossible for months thereafter to give attention to the reduction of the data." The data, when finally reduced, led to a value for Planck's constant of 6.57×10^{-34} joule-sec.

Emergence of quantum physics

2. Photoelectric effect

- Photoelectric effect– the ejection of electrons from a surface by the action of light (Hertz (1887))

- Classical laws explanation → electrons should be emmited with energy proportional to the light intensity

- Thus, The magnitude of the current is proportional to the light intensity

- Observation → The energy of the electrons emmited does not depend on the light intensity; it depends on linearly with the frequency of the incident light

Emergence of quantum physics

2. Photoelectric effect

- Classical EM theory does not explain the frequency dependence for the emissions
- Einstein (1905) , generalised Planck's idea (light interacting with matter reveals quantum behaviour at low energies)
- Now, all lights exists in quanta
- He assumed that electrons needs a definite amount of energy to escape the metal
- Light with a given frequency (υ) incids on a metal with a given number of quanta, each with energy hυ
- Them quanta would collide with the electrons providing them the energy necessary to escape from the metal

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2. Photoelectric effect

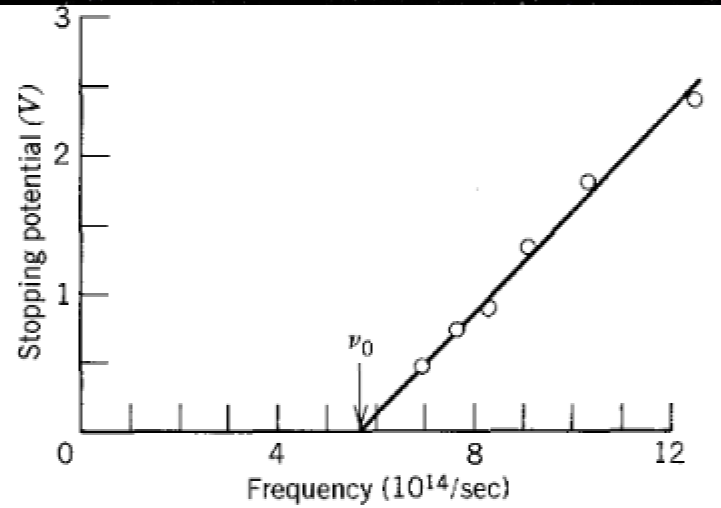

Figure 2-3 The stopping potential at various frequencies for sodium. The points show Millikan's data, except that the correction mentioned in the caption to Figure 2-1 has been recalculated using a recent measurement of the contact potential. The cutoff frequency ν_0 is 5.6×10^{14} Hz.

Einstein (1905) → $$\frac{1}{2}mV^2 = hv - W$$

W → energy needed to separate the elctrons from the metal (work function)

Emergence of quantum physics

3. Compton effect

- Einstein’s proposal that the quanta of energy should also manifest outside the blackbody cavity explained the photoelectric effect
- However, this did not lead him to the notion of the quantum of radiation as a particle
- Einstein (1916) analising the concept of gas of quanta was led to the prediction that the quanta of light (photons) carries momentum and energy

Emergence of quantum physics

3. Compton effect

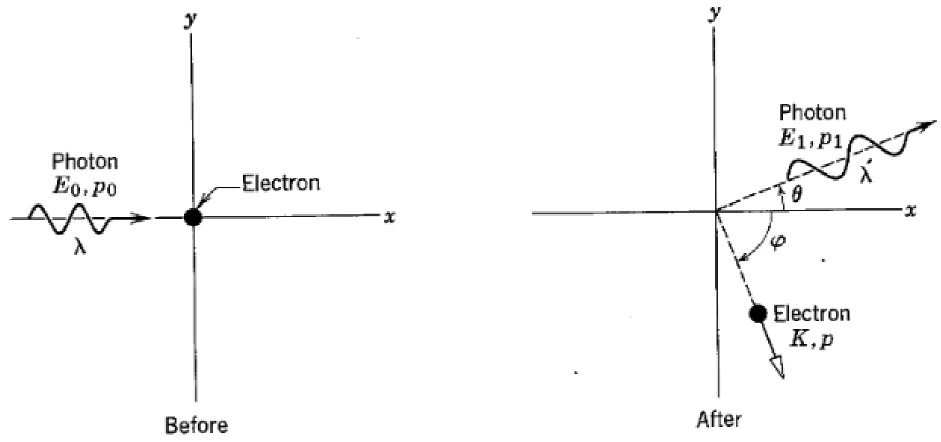

Figure 2-7 Compton's interpretation. A photon of wavelength λ is incident on a free electron at rest. On collision, the photon is scattered at an angle θ with increased wavelength λ', while the electron moves off at angle φ.

- Compton wavelenght of the electron (1923-24)

$$\frac{h}{m_e c} = 2.426 \times 10^{-12} m$$

Emergence of quantum physics

4. Bohr’s atom

- The discovery of electrons (Thomson), x-rays (Rontgen), radioactivity (Becquerel & Curies), provided the tools for a better understanding of the structure of the atom

- Thomson’s model → By 1897 he measured the ratio of charge to the mass of the electron

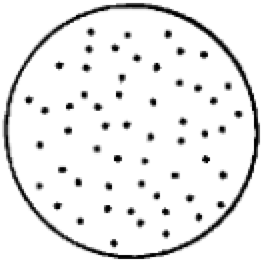

Figure 4-1 Thomson’s model of the atom—a sphere of positive charge embedded with electrons.

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4. Bohr’s atom

- Inadequacy was proved by experiments

Prediction→

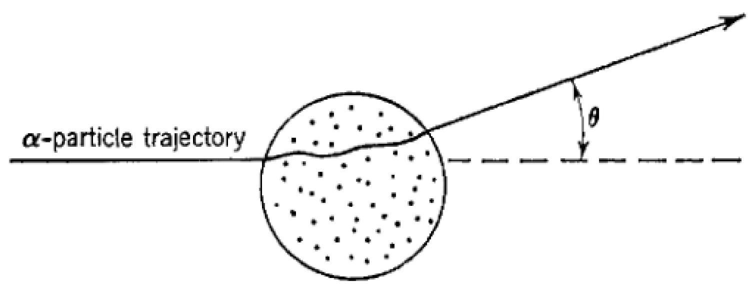

Figure 4-3 An α particle passing through a Thomson model atom. The angle θ specifies the deflection of the α particle.

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4. Bohr's atom

- Inadequacy was proved by experiments

Observation →

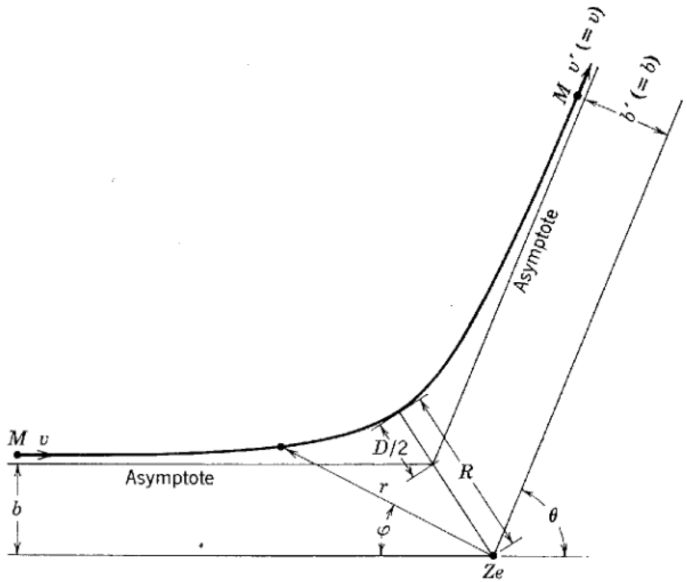

Figure 4-4 The hyperbolic Rutherford trajectory, showing the polar coordinates r, φ and the parameters b, D. These two parameters completely determine the trajectory, in particular the scattering angle θ and the distance of closest approach R. The nuclear point charge Ze lies at a focus of the branch of the hyperbola.

Emergence of quantum physics

4. Bohr’s atom

Rutheford → The positively charged nucleus attracts the negatively charged electrons and the force law has a behaviour

$$^{1}/_{r^2}$$

The electrons travel in circular or elliptic orbits about the nucleus

Emergence of quantum physics

4. Bohr’s atom

<u>PROBLEMS</u> (Rutheford model)

Classical electrodynamics tell us that an accelerating charge radiates

Thus an electron in orbit loses energy

It can be estimate that it would take about 10^{-10}s to spiral into the nucleus of $10^{-10}\mathrm{m}$

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4. Bohr's atom

Classical electrodynamics was unable to explain the atomic spectra known by that time

The information about the spectra of the hydrogen atom can be summarized by this formula

$$k = R_H \left(\frac{1}{nf^2} - \frac{1}{ni^2} \right)$$

The observed spectral lines are due to the electron making transitions between energy levels in an atom

Table 4-1 The Hydrogen Series

Names	Wavelength Ranges	Formulas	
Lyman	Ultraviolet	$\kappa = R_H \left(\frac{1}{1^2} - \frac{1}{n^2} \right)$	$n = 2, 3, 4, \ldots$
Balmer	Near ultraviolet and visible	$\kappa = R_H \left(\frac{1}{2^2} - \frac{1}{n^2} \right)$	$n = 3, 4, 5, \ldots$
Paschen	Infrared	$\kappa = R_H \left(\frac{1}{3^2} - \frac{1}{n^2} \right)$	$n = 4, 5, 6, \ldots$

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4. Bohr's atom

BOHR POSTULATES (1913)

1. An electron in an atom moves in a circular orbit about the nucleus under the influence of the Coulomb attraction between the electron and the nucleus, obeying the laws of classical mechanics (CM)
2. Instead of the <u>infinity of orbits</u> which would be possible in CM, it is only possible for an electron to move in an orbit for which its orbital angular momentum L is a multiple of h → $L = n\hbar$
3. Despite the fact that it is constantly accelerating, an electron moving in such an allowed orbit does not radiate electromagnetic (EM) energy. Thus, its total energy E remains constant.
4. EM radiation is emitted if an electron, initially moving in an orbit of energy E_i, changes its motion to move in an orbit of energy E_f . The frequency of the emitted radiation υ is equal to the quantity

$$h\,\upsilon = E_i - E_f \quad (E_i > E_f)$$

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4. Bohr’s atom

With Bohr model of the atom physicists were able to calculate in great detail many of the spectroscopy results obtained by experimenters of previus decades

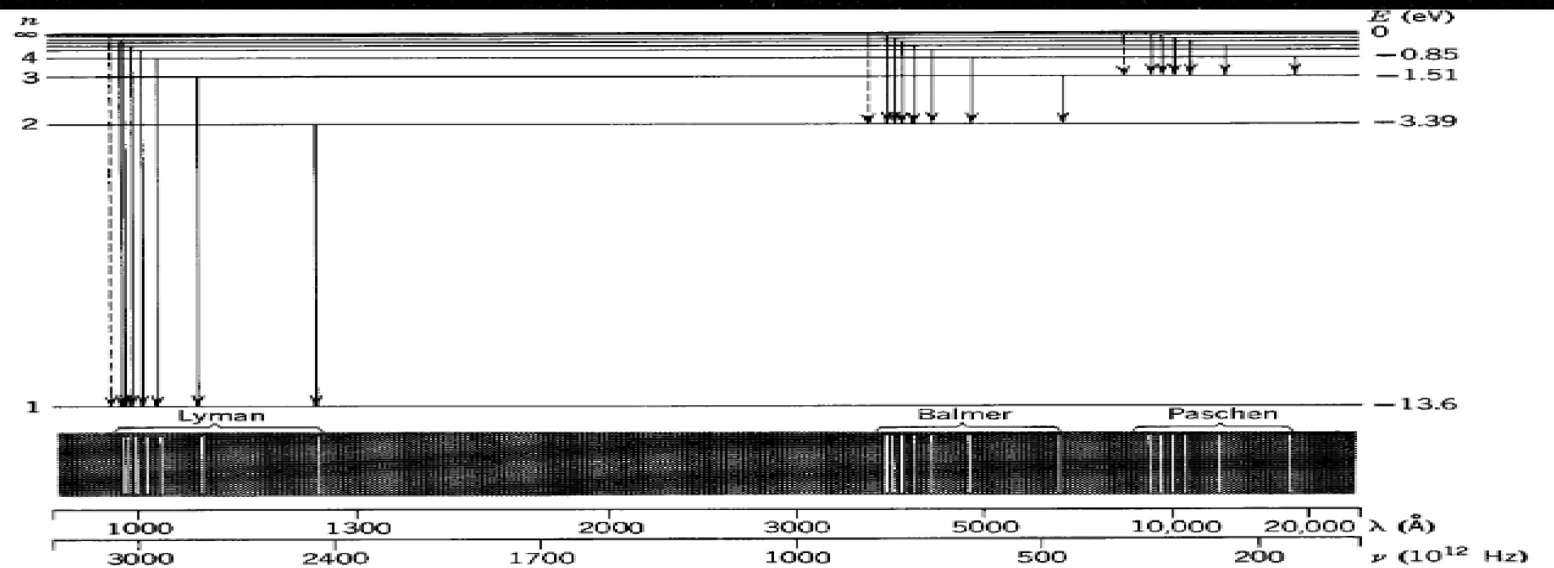

Figure 4-12 *Top:* The energy-level diagram for hydrogen with the quantum number n for each level and some of the transitions that appear in the spectrum. An infinite number of levels is crowded in between the levels marked $n = 4$ and $n = \infty$. *Bottom:* The corresponding spectral lines for the three series indicated. Within each series the spectral lines follow a regular pattern, approaching the series limit at the shortwave end of the series. As drawn here, neither the wavelength nor frequency scale is linear, being chosen as they are merely for clarity of illustration. A linear wavelength scale would more nearly represent the actual appearance of the photographic plate obtained from a spectroscope. The Brackett and Pfund series, which are not shown, lie in the far infared part of the spectrum.

Emergence of quantum physics

4. Bohr's atom

Bohr atomic model was na enormous success and a big step forward

However, it is important to note that this is the simplest quantum model of the atom and more sofisticated tools were still necessary!!

Emergence of quantum physics

5. de Broglie and matter waves

- de Broglie (1923) suggested that the dual wave-particle nature of radiation should have its counterpart dual wave-particle nature of matter
- Particles should also have wave properties
- Wavelenght associated to the particles

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

Emergence of quantum physics

5. de Broglie and matter waves

Comparison of an x-ray diffraction pattern and an electron diffraction pattern

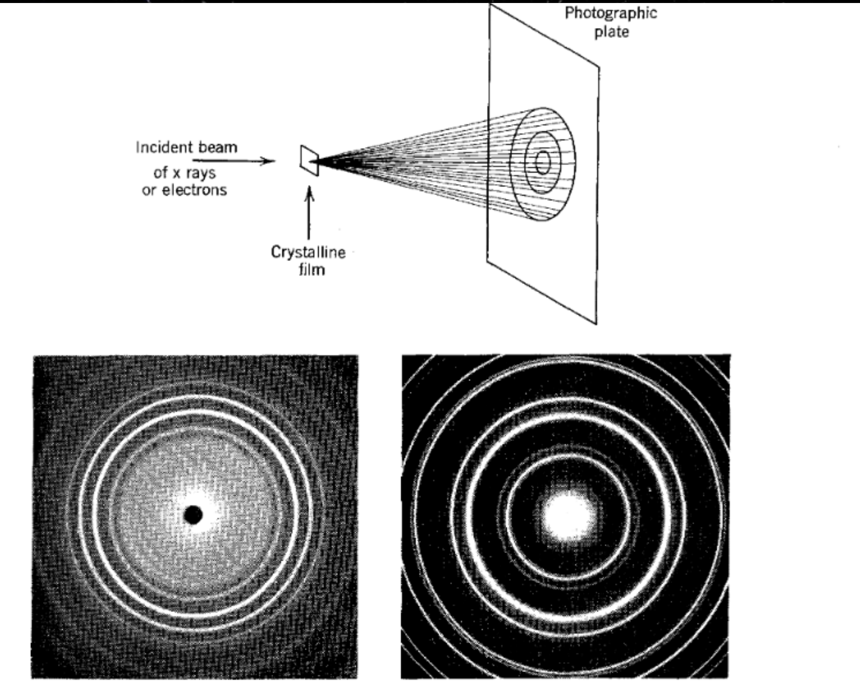

Figure 3-4 *Top:* The experimental arrangement for Debye-Scherrer diffraction of x rays or electrons by a polycrystalline material. *Bottom left:* Debye-Scherrer pattern of x-ray diffraction by zirconium oxide crystals. *Bottom right:* Debye-Scherrer pattern of electron diffraction by gold crystals.

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5. de Broglie and matter waves

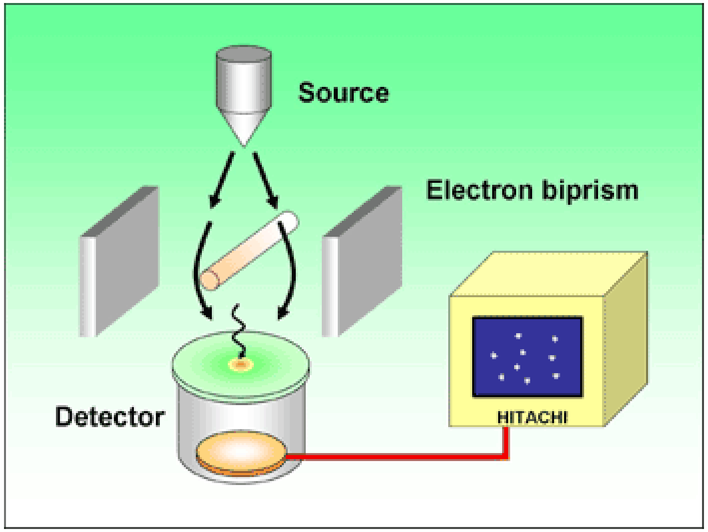

Fig. 1 Double-slit experiment with single electrons

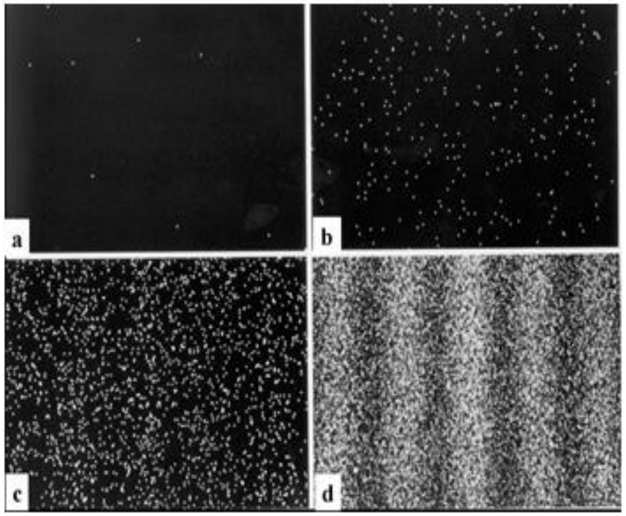

Fig. 2 Single electron events build up to from an interference pattern in the double-slit experiments.

https://www.hitachi.com/rd/research/materials/quantum/doubleslit/index.html

Emergence of quantum physics

5. de Broglie and matter waves

- J. J. Thomson(1897)discovered the electron (which he characterized as a particle with a definite charge-to-mass ratio) was awarded the Nobel Prize in 1906
- G. P. Thomson, JJ's son, in 1927 discovered electron diffraction and was awarded the Nobel Prize (with Davisson) in 1937.

"One may feel inclined to say that Thomson, the father, was awarded the Nobel Prize for having shown that the electron is a particle, and Thomson, the son, for having shown that the electron is a wave."

Max Jammer

Emergence of quantum physics

6. Heisenberg picture and uncertainty relation

- Starting point (1925)→ The only sensible way to formulate the mechanics of the system is *observing it*
- By *'observation'* we mean any interaction experienced by the system, such as scattering off it of light or an electron
- In the absence of interaction the system would be tottaly isolated from the outside world
- Only by some form of interaction the system exists in a definite state
- Heisenberg uncertanty principle results from the realisation that any act of observation on the quantum system will disturb it

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6. Heisenberg picture and uncertainty relation

The photon wavelenght is related to its momentum by

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

The greater photon’s momentum the shorter the wavelenght and vice-versa

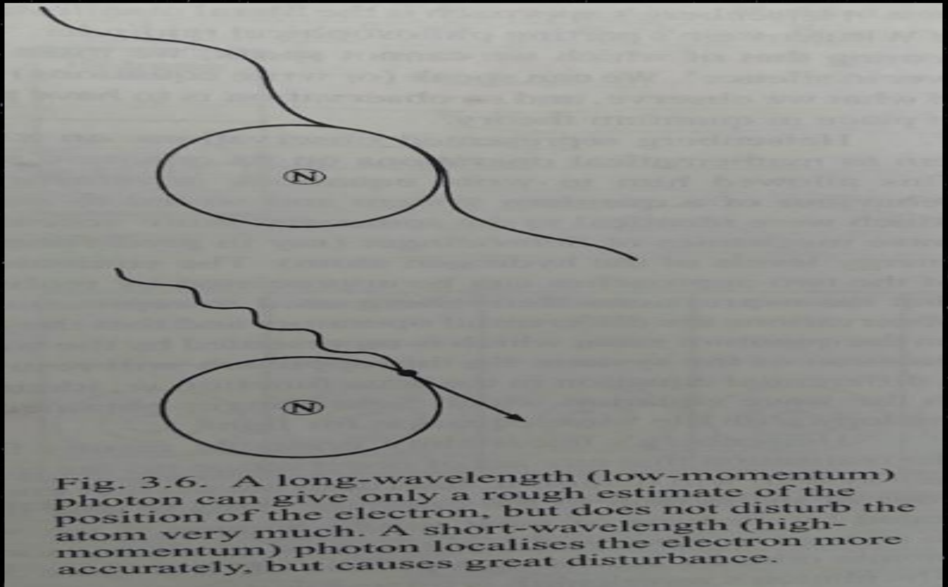

Fig. from the book:
The ideas of particle physics
By Coughlan, Dodd, Gripaios

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6. Heisenberg picture and uncertainty relation

Use photons to hightest possible momentum (shortest wavelenght) to determine accurately the electron position

However the electron will be disturbed by the high momenton of the photon and so its momentum will be very uncertain

The essence of the Heisenberg uncertain principle:

Knowledge of one parameter implies uncertain of the other conjugate parameter

$$\Delta p \Delta x \geq \frac{\hbar}{2}$$

Emergence of quantum physics

7. Stern-Gerlach experiment

- In 1922 Stern and Gerlach measured the values of the magnetic dipole moment for silver atoms by sending a beam of them through a nonuniform magnetic field.

Neutral atoms, the only net force acting on them is

$$\boldsymbol{F}_z = \frac{\partial \boldsymbol{B}_z}{\partial z}\mu_{lz}$$

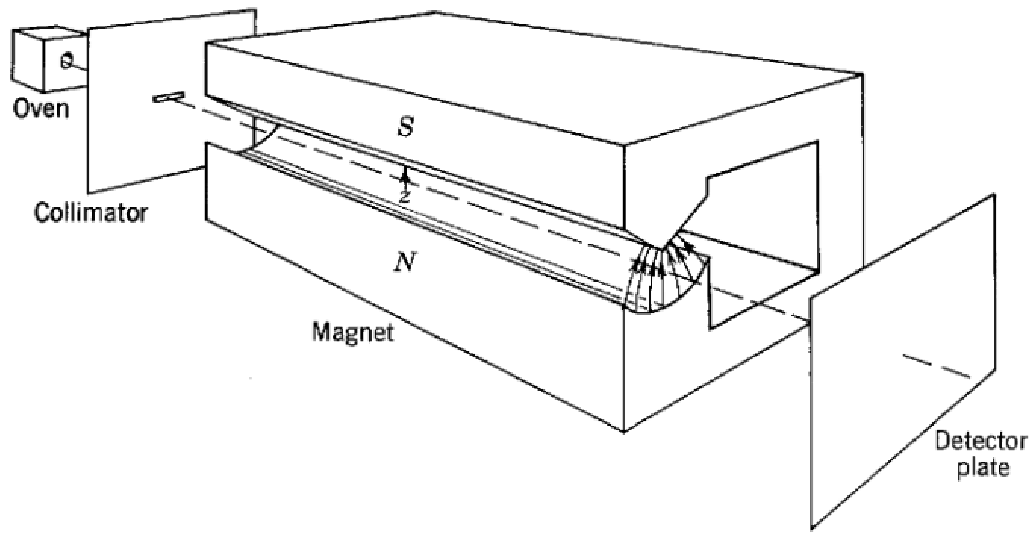

Figure 8-5 The Stern-Gerlach apparatus. The field between the two magnet pole pieces is indicated by the field lines drawn at the near end of the magnet. The field intensity increases most rapidly in the positive z direction (upward).

7. Stern-Gerlach experiment

- Since the force acting on each atom of the beam is proportional to the value of μ_{lz}, each atom is deflected by magnetic field by an amount proportional to μ_{lz}.
- Thus the beam is analyzed into components according to the various values of μ_{lz}.
- The deflected atoms strike a metallic plate, upon which they condense and leave a visible trace.
- If the orbital magnetic moment vector of the atom has a magnitude μ_l, then in classical physics the z component μ_{lz} of this quantity can have any value from

$$-\mu_{lz} \quad \text{to} \quad +\mu_{lz} .$$

- The reason is that classically the atom can have any orientation relative to the z axis

Emergence of quantum physics

7. Stern-Gerlach experiment

- The predictions of QM is that μ_{lz} must have discrete quantized values

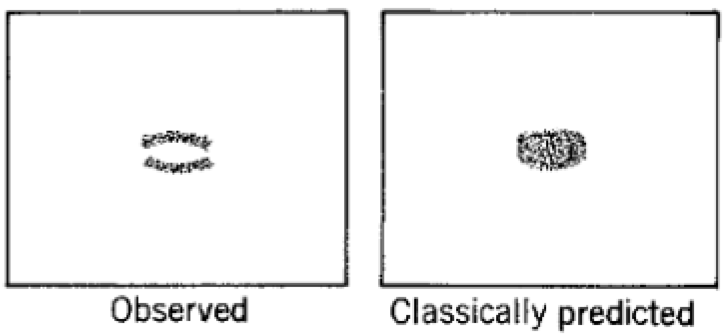

Figure 8-6 The deflection pattern recorded on the detecting plate in a Stern-Gerlach measurement of the *z* component of the magnetic dipole moment of silver atoms. Maximum deflection occurs at the center of the beam because the atoms there pass through the region of maximum field gradient, $\partial B_z/\partial z$. The observed pattern consists of two discrete components due to space quantization. According to the classical prediction a continuous band would be expected.

- μ is proportional to the angular momentum (L). The experimental results suggests that the L is quantized

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Emergence of quantum physics

8. Wave function and Schrodinger equation

- Following de Broglie, Schrodinger (1926) developed the idea of particle waves into a wave mechanics proper

- The starting point was a wave equation that describs the behaviour of light waves in space and time

- He described a matter wave equation that represents the behaviour of matter

- Schrodinger’s equation describes a particle by its wave function ($\psi(x, t)$) and shows how the particle wavefunction evolves in space and time under specific set of curcunstances

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

8. Wave function and Schrodinger equation

The arguments that guided him to this equation are basically:

1. It must be consistent with the de Broglie ideas → $\lambda = h/p$, $v = E/h$

2. It must be consistent with the equation classical equation → $E = p^2/2m + V$

3. It must be linear in $\psi(x, t) = c_1\psi_1(x,t) + c_2\psi_2(x,t)$

This linearity requirement ensures that we shall be able to add together wave functions to produce the constructive and destructive interferences that are so characteristic of Waves

4. The potential energy V is in general a function of x and t. However, there is a special case where $V(x,t) = V$ → This is just the case of the free particle

Emergence of quantum physics

8. Wave function and Schrodinger equation

Born Interpretation (1926)

- The wave function of quantum mechanics is complex

- This is in contrast to waves in classical mechanics. For instance, a wave in a string can be specified by one real function which gives the displacement of the string

- The fact that wave functions are complex makes it apparent that we should not attempt to give to wave functions a physical existence in the same sense that water waves have a physical existence.

Emergence of quantum physics

8. Wave function and Schrodinger equation

Born Interpretation (1926)

- The basic connection between the properties of the wave function $\psi(x,t)$ and the behavior of the associated particle is expressed in terms of the probability density P(x,t).

$$P(x,t) = \psi^*(x,t)\psi(x,t)$$

This quantity specifies the probability, per unit length of the x axis, of finding the particle near the coordinate x at time t

Emergence of quantum physics

8. Wave function and Schrodinger equation

Born Interpretation (1926)

- Since the motion of a particle is connected with the propagation of an associated wave function (the de Broglie condition), these two entities must be associated in space.

- That is, the particle must be at some location where the waves have an appreciable amplitude. Therefore P(x,t) must have an appreciable value where $\psi(x,t)$ has an appreciable value

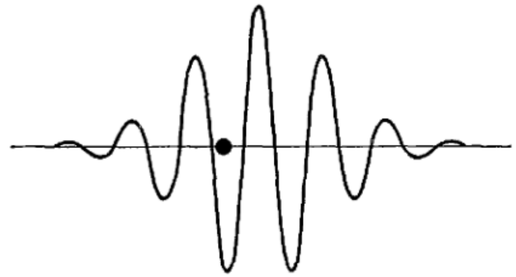

Figure 5-2 A very schematic picture of a wave function and its associated particle. The particle must be at some location where the wave function has an appreciable amplitude.

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Emergence of quantum physics

8. Wave function and Schrodinger equation

- With Schrodinger equation, we are able to show that the electron wave function can assume only certain discrete energy levels
- These energy levels are the same as the energies of electronic orbits of the hidrogen atom postulated by Bohr
- The particle wavefunction is na extremely significant concept which we shall use frequently during the course

Emergence of quantum physics

8. Wave function and Schrodinger equation

HYDROGEN ATOM

$$\left(-\frac{\hbar^2}{2\mu}\nabla^2 - \frac{e^2}{4\pi\varepsilon_0 r}\right)\psi(r,\theta,\varphi) = E\psi(r,\theta,\varphi)$$

Schrodinger equation

$$\psi_{n\ell m}(r,\theta,\varphi) = \sqrt{\left(\frac{2}{na_0^*}\right)^3 \frac{(n-\ell-1)!}{2n(n+\ell)!}} e^{-\rho/2}\rho^\ell L_{n-\ell-1}^{2\ell+1}(\rho) Y_\ell^m(\theta,\varphi)$$

Solution

n = 1, 2, 3, ...; l = 0, 1, ...n-1; m = -l,...,l

$$\rho = \frac{2r}{na_0^*},$$

$$a_0^* = \frac{4\pi\varepsilon_0\hbar^2}{\mu e^2},$$

Emergence of quantum physics

8. Wave function and Schrodinger equation

- Phipps and Taylor (1927), used the Stern-Gerlach technique on a beam of hydrogen atoms

- Concluded that an electron has an intrinsic magnetic dipole moment μ_s , due to the fact that it has an intrinsic angular momentum S called spin.

s = ${}^{-1}/_{2}$, ${}^{+1}/_{2}$ (Pauli exclusion principle)

- Schodinger equation

- It does not include spin
- It is not relativistic

- Dirac Equation

COMING NEXT …

- Mathematical tools of Quantum Mechanics
- Postulates of Quantum Mechanics
- Quantum Computers – Physical Realization