# Quantum Mechanics Introduction

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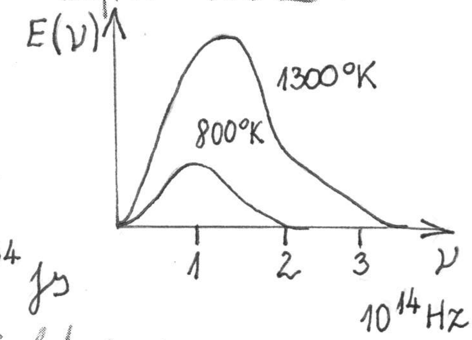
Physics Vol. III.

- Black body radiation

$\frac{1}{V} E(\nu)\, d\nu$

Planck: material → oscillators
abs. & em. in $E = h\nu$ quanta



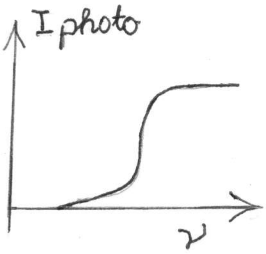

$$E(\nu) = \frac{8\pi h \nu^3}{c^3} \frac{1}{e^{h\nu/kT} - 1} \qquad h = 6{,}6 \cdot 10^{-34}\ Js$$

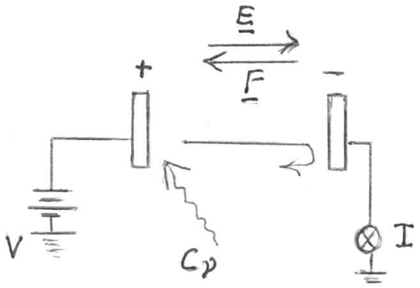
Wien: $\lambda_{max} \cdot T = \text{const.}$

Stefan - Boltzm.:

$$\int_0^\infty E(\nu)\, d\nu = \sigma T^4$$

- Photoelectric effect



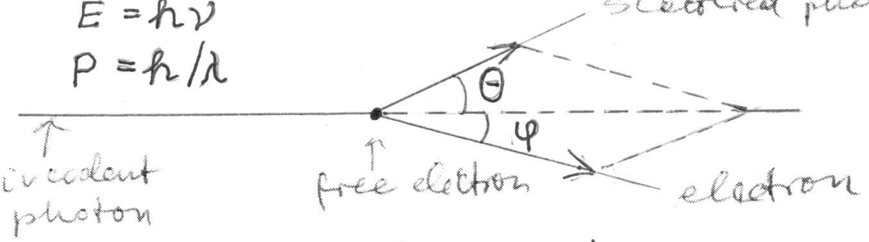

$I = 0$ at $V = V_0$

$eV_0 = E_{kin.max} = h\nu - \phi$

$\phi$ = work function

- Compton effect

$E = h\nu$
$p = h/\lambda$




$E' = h\nu'$
$p' = h/\lambda'$

$$\lambda' - \lambda = \lambda_c (1 - \cos\Theta)$$

Calculating as collision /conservation of energy and momentum/

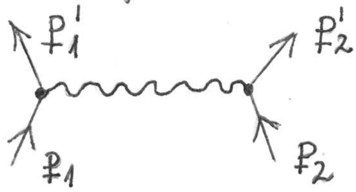
$$\lambda_c = \frac{h}{m_e \cdot c}$$

$$\left.\begin{aligned} &\text{Maxwell: } E = c \cdot p \\ &\text{relativity: } E = c\sqrt{m_0^2 c^2 + p^2} \end{aligned}\right\} \to m_0 = 0$$

– Photons

$E = h\nu$, $p = \frac{h}{\lambda}$ Description of interaction of electromagnetic waves with charged particles with a photon of energy $E$, momentum $p$

In general: electromagnetic interaction ≡ exchange of photons between charged particles




– Stationary states

System of charged particles: atom, molecule, nucleus etc.

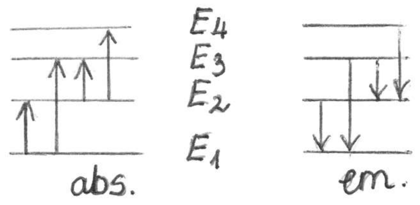
- resonance frequencies
- absorption spectrum
- ground state, excited states
- absorption frequencies = emission frequencies

Bohr: Transition between states with energies $E$ and $E'$ $h\nu = E' - E$

Discreet energy levels → stationary states

$A + h\nu \longrightarrow A^*$ abs.

$A^* \longrightarrow A + h\nu$ em.

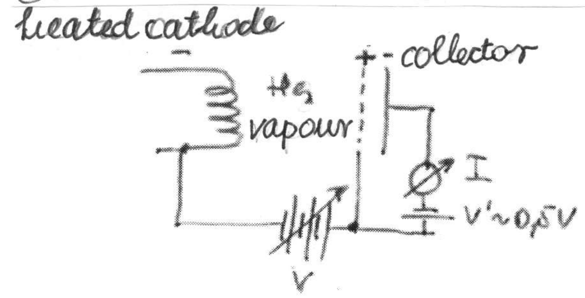


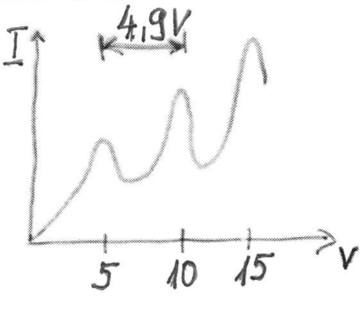

– Contradiction with classical mechanics

quantization of energy

electron circulates but does not radiate

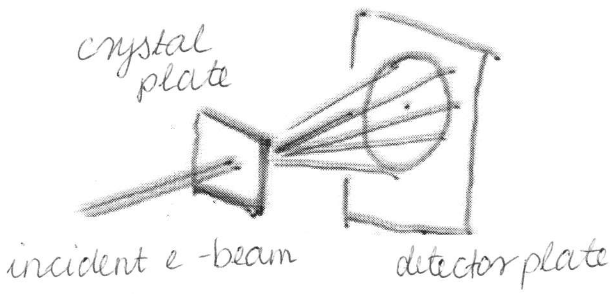
Franck-Hertz experiment

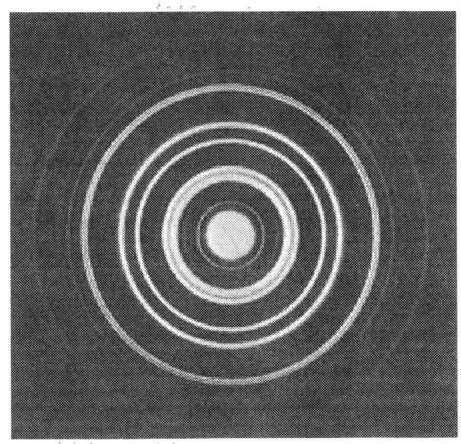


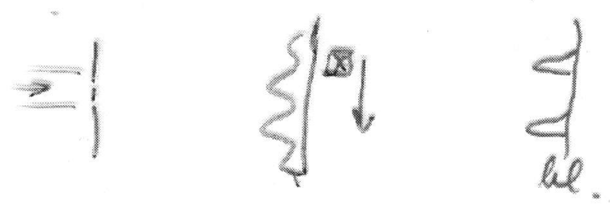
- Wave particle duality

Electrons may behave like waves: interference, diffr.



Diffraction image (powdersample)



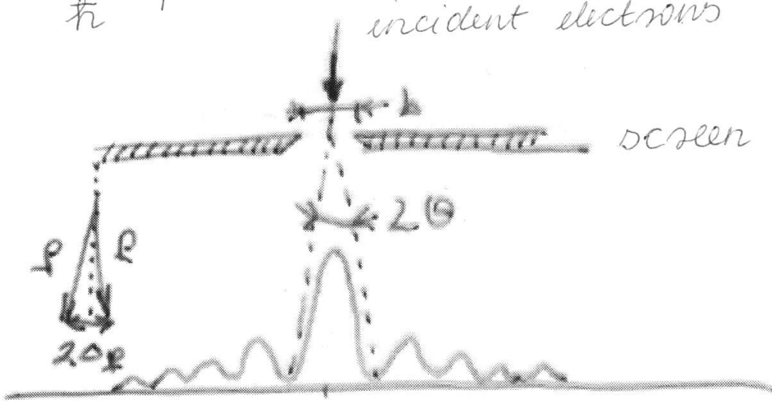
$\lambda = \frac{h}{p}$ de-Broglie wavelength

Free particle → wave packet

- Heisenberg uncertainty relationship

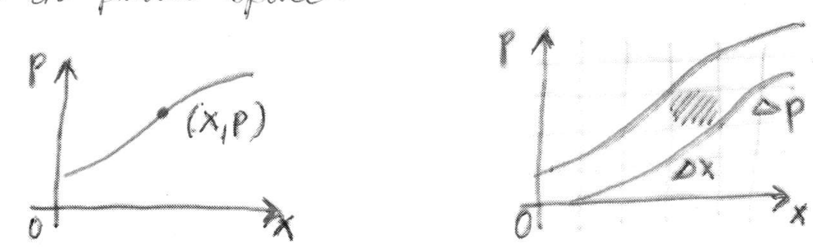
Wave packet → Fourier transform $\Delta x \cdot \Delta k \approx 2\pi$

$\Delta k = \frac{1}{\hbar} \Delta p \rightsquigarrow \Delta x \Delta p \sim h$




Diffraction image intensity distribution

Motion in phase space:




Energy - time

$\Delta t \cdot \Delta E \sim h$ / Fourier tr. of wave packet

$\Delta t \cdot \Delta \omega \sim 2\pi \qquad \Delta \omega = \frac{\Delta E}{\hbar}$

Stationary state → lifetime → linewidth

Wave function, probability density, Schrödinger equation (4.)

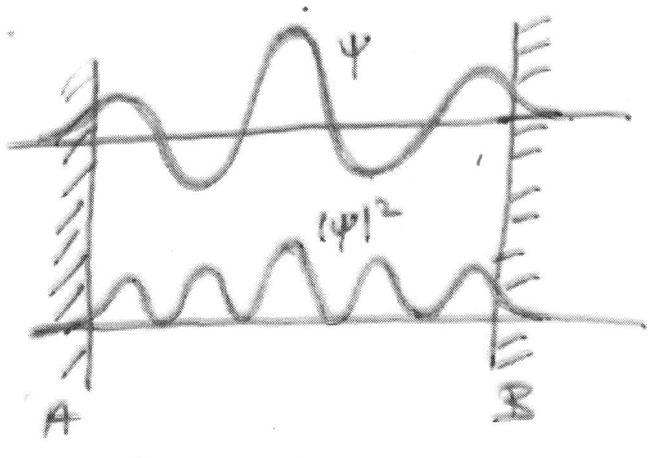
- Motion of particles
  Classical orbit ↓
  Localized particle – standing wave – wavefunction $\psi(x)$
  Wave intensity $\sim |\psi|^2$
  $\psi$ complex $\psi^*$ compl. conjugate $|\psi|^2 = \psi^* \psi$

Probability of finding the particle in a range $\Delta x$ around $x \equiv |\psi(x)|^2 dx$

In three dimension, Volume

$$P_V = \int_V |\psi(x,y,z)|^2 dx\,dy\,dz$$

$$\int_{\text{whole space}} |\psi|^2 dx\,dy\,dz = 1$$




particle moves between A and B

E.g.: Probability distribution of electron position in an atom

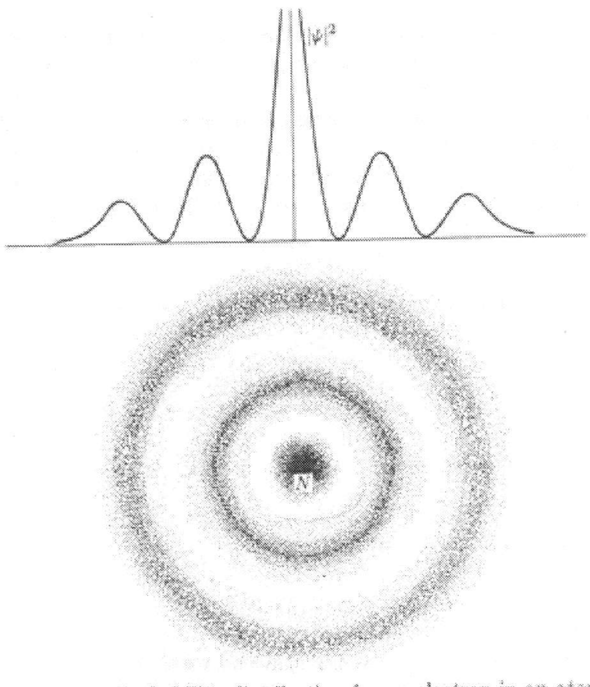



Fig. 2–2. Probability distribution for an electron in an atom.

- Question: how to determine $\psi$?
  Depends on the forces acting on the particle as well as on the energy of the particle
  Full energy: $E = \frac{p^2}{2m} + E_p \Leftarrow$ forces

Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + E_p(x)\psi = E\psi$$ (1 dim., m = particle mass)

Intuitive derivation:

1 dim. wave equation: $\frac{d^2\xi}{dx^2} + k^2\xi = 0$ (in general)

$k = \frac{2\pi}{\lambda}$ wave number $\quad p = \hbar k$ in quantum mech.

writing this to the wave equation:

$$\frac{d^2\psi}{dx^2} + \frac{p^2}{\hbar^2}\psi = 0$$

but from the full energy $E \rightsquigarrow p^2 = 2m[E - E_p]$

with this $\quad \frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}[E - E_p(x)]\psi = 0$

- Solutions

  E.g. $\psi(x) = e^{ikx} \rightarrow |\psi|^2 = 1$ : since $\Delta p = 0 \rightsquigarrow \Delta x \rightarrow \infty$

  Principle of superposition ↑: $\psi_1$ and $\psi_2$ solution $\rightsquigarrow$

  $\psi = a\psi_1 + b\psi_2$ — " —

  $p = \hbar k$, $E = \frac{\hbar^2 k^2}{2m}$ particle moving $+x$ dir. $e^{ikx}$

  — " — — " — $-x$ dir. $e^{-ikx}$

  $\psi_1 = a \cdot e^{ikx} \qquad \psi_2 = a\, e^{ik(x+b)}$

  $\psi = \psi_1 + \psi_2$

  $|\psi|^2 = 2a^2(1 + \cos kb)$ — interference

  Concrete solutions $\rightarrow$ boundary conditions ($E_p(x)$)

Quantum mechanics /3.

Potential step, potential box, harmonic oscillator, tunneling effect

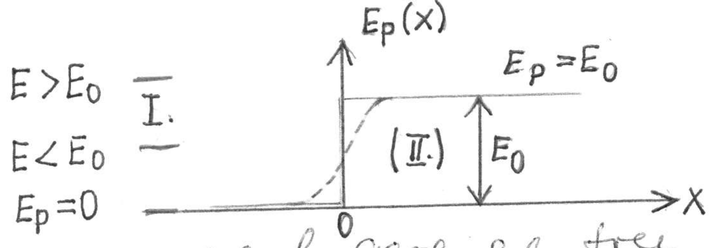


— Potential step

$E_p(x) \rightarrow$

$E_p(x) = 0; \quad x < 0$

$E_p(x) = E_0; \quad x > 0$




- - - real case, e.g. free electrons in a metal near the surface

From the Schrödinger eq.: $\psi(x)$

a, $\underline{E < E_0}$

kinetic energy $E_k = E - E_0 < 0$ would be, when $x > 0$

$\rightsquigarrow$ particle can not enter $x > 0$

$\underset{\sim\sim}{\text{I.: } x < 0}$ $\quad E_p = 0 \quad$ Schr.: $\dfrac{d^2\psi_1}{dx^2} + \dfrac{2mE}{\hbar^2}\psi_1 = 0$

$\psi_1 = Ae^{ikx} + Be^{-ikx}$ $\quad$ ($e^{-ikx} \rightarrow$ reflected particle)

$\underset{\sim\sim}{\text{II.: } x > 0}$ $\quad E_p = E_0 \quad$ Schr.: $\dfrac{d^2\psi_2}{dx^2} + \dfrac{2m(E-E_0)}{\hbar^2}\psi_2 = 0$

Introduce $\alpha^2 = \dfrac{2m(E_0 - E)}{\hbar^2}$

Schr. $\dfrac{d^2\psi_2}{dx^2} - \alpha^2\psi_2 = 0$

Solution: $e^{\pm\alpha x}$ $\quad$ but $e^{+\alpha x}$ would give particle in region II.

$\psi_2(x) = C'e^{-\alpha x}$

Surprising: $\psi_2(x) \neq 0 \rightarrow$ particle enters even if $E < E_0 \rightarrow$ no sharp boundary

Penetration is not very deep (fast decay)

Factors A, B, C from the continuity of $\psi$ at $x = 0$

$\psi_1 = \psi_2$ and $\frac{d\psi_1}{dx} = \frac{d\psi_2}{dx}$ at $x=0 \rightsquigarrow$

$A + B = C$ and $ik(A-B) = -\alpha C$ from this

$\psi_1(x) = A\left(e^{ikx} + \frac{ik+\alpha}{ik-\alpha} e^{-ikx}\right)$, $\psi_2(x) = \frac{2ik}{ik-\alpha} A e^{-\alpha x}$

Incident intensity: $|\psi_{in}|^2 = |A|^2$

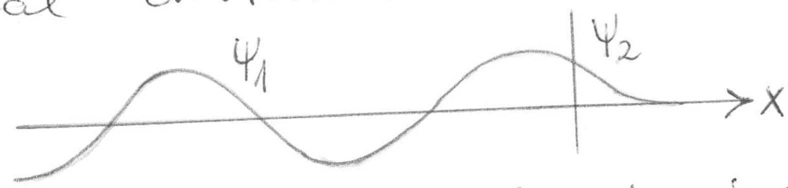
Reflected intensity: $|\psi_{refl.}|^2 = |B|^2 = \left|\frac{ik+\alpha}{ik-\alpha} A\right|^2 = |A|^2$

$\rightsquigarrow$ All particles are reflected even those that slightly penetrate region II.

$\psi_1(x)$ can be rewritten

$= \frac{2ik}{ik-\alpha} A\left(\cos kx - \frac{\alpha}{k} \sin kx\right)$

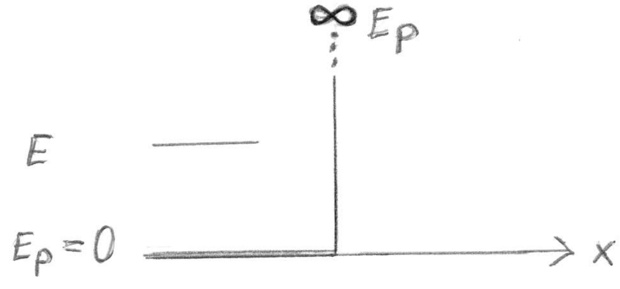
Spatial distribution of the real part of $\psi_1$ and $\psi_2$

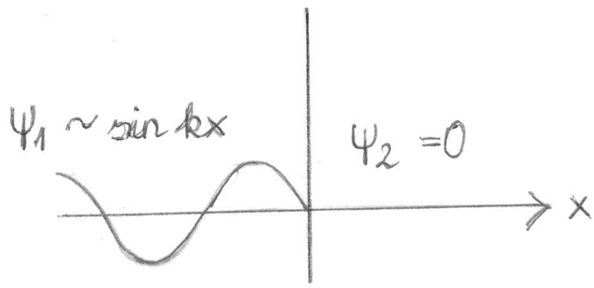



When the height of the step increases ($E_0$ increases)

$\rightsquigarrow \alpha$ increases $\psi_2$ decays faster

$E_0 - \infty$



b. $E > E_0$

classically: the particle moves through, only slightly slows down at $x = 0$

Region I: $\psi_1 = Ae^{ikx} + Be^{-ikx}$ solution

Region II: $k'^2 = \frac{2m(E-E_0)}{\hbar^2}$ with this

$$\frac{d^2\psi_2}{dx^2} + k'^2\psi_2 = 0$$

Since all the particles move on

$$\psi_2(x) = C'e^{ik'x}$$

$A + B = C$ and $k(A-B) = k'C$ from the boundary conditions

Interesting: $B \neq 0 \rightarrow$ Reflection $\neq 0$