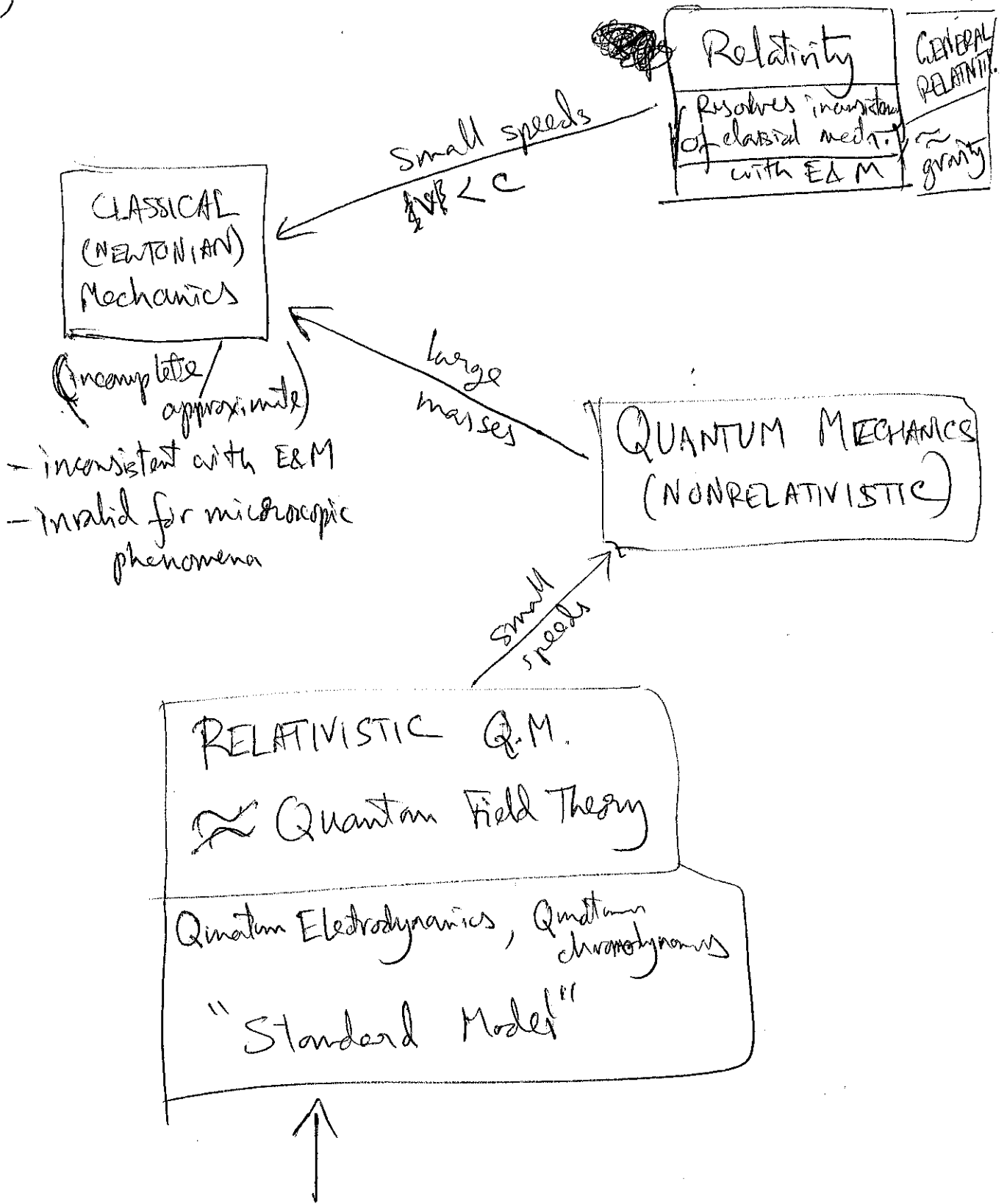


1



Still incomplete &
Does not incorporate gravity

- * QM is less intuitive than Classical Mech, E&M
- * Many new concepts, some confusing ["Nobody understands QM"]
- * ~~First~~ First few (~6) classes: ~~initial~~ broad overview, ~~intro~~ intro to several concepts/sys, historical introduction, etc.

* ~~Fundamental~~ Fundamental ~~equation/law~~ of Newtonian Mechanics: (one particle)

$$F = ma \quad \text{or} \quad -\frac{\partial V}{\partial x} = m \frac{d^2 x}{dt^2} \quad 1D$$

$$\vec{F} = m\vec{a} \quad \text{or} \quad -\vec{\nabla} V = m \frac{d^2 \vec{r}}{dt^2} \quad 3D$$

1D means: the particle is constrained to

move along the x-direction.

→ If you know $x(0), \dot{x}(0)$, you can calculate $\begin{cases} x(t) \\ \dot{x}(t) \end{cases}$

→ can be generalized: ~~to N particles~~

to ~~N~~ $N \geq 1$ particles; one eq. for each pcle

to constrained motion. (Lagrangian mechanics)

→ Impossible to prove Newton's laws;

we believe it because it keeps explaining

physical phenomena, ~~in~~ in its regime

of applicability (macroscopic objects, "slow" speeds)

③

* Fundamental equation of QM: Schrödinger Eq.

~~General~~ General form: $\hat{H}\Psi = i\hbar \frac{\partial \Psi}{\partial t}$

Here $\hbar = \frac{h}{2\pi}$ and $h \approx 6.63 \times 10^{-34}$ J·s

is PLANCK'S CONSTANT

* Ψ is the wavefunction or state vector,

describes the state of the system.

→ SOMETIMES A FUNCTION, SOMETIMES A "VECTOR"!!

* \hat{H} is the Hamiltonian operator.

* Example: ^{single} particle in 1D:

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

• In this case, $\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$

\uparrow
(kinetic energy operator)

\uparrow
(potential energy operator)

- Ψ has been written as function of x and t

- The SE doesn't give x as a function of t , unlike in classical mechanics.
- Instead, $|\Psi(x,t)|^2$ gives the probability density for finding the particle at position x at time t .
- In QM, probabilistic knowledge of physical variables.

~~A class of solutions~~
~~the form of the SE are~~

* The ^{important} class of solutions to SE are stationary solutions
 For 1 pde in 1D,
 $\Psi(x,t) = \psi(x) e^{-iEt/\hbar}$

Substituting in SE gives

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V(x)\psi(x) = E\psi(x)$$

→ Time-independent Schrödinger equation.

⑤

* $\hat{H} \psi(t) = i\hbar \frac{\partial}{\partial t} \psi(t)$ Time-dependent Schr. Eq. (TDSE)

Using $\psi(t) = \psi e^{-iEt/\hbar}$,

$\hat{H} \psi = E \psi$ Time-independent Schr. Eq.

* We'll study both ~~time-dependent and time-independent~~ in detail.

* Example: Spin- $\frac{1}{2}$ object (electron/proton/singly-charged ion) fixed in space

ψ has no spatial dependence.

Can be expressed as a two-component "vector"

$\psi(t) = u(t) |\uparrow\rangle + v(t) |\downarrow\rangle$

$\psi(t) = \begin{pmatrix} u(t) \\ v(t) \end{pmatrix}$

u, v can be complex

$|\uparrow\rangle =$ state where spin points in $+z$ direction ⑥
 $|\downarrow\rangle =$ " " " " " $-z$ "

In this case, Hamiltonian operator is 2×2 matrix, TDSE ^($H\psi = i\hbar \frac{\partial \psi}{\partial t}$) has the form:

$$\begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \begin{pmatrix} u(t) \\ v(t) \end{pmatrix} = i\hbar \begin{pmatrix} \frac{\partial u}{\partial t} \\ \frac{\partial v}{\partial t} \end{pmatrix}$$

TIME-INDEP form from p. 11

* Looks very different from the case of particles on the x -axis?

* ~~The~~ The difference is in the dimension of HILBERT SPACE.

* The wave functions (state vectors) are members of a vector space called Hilbert space. * If Hilbert space is D dimensional, wavevector ~~has~~ has D complex ~~components~~ components.

\uparrow
 different from Euclidean vectors.

* Two-state (spin- $\frac{1}{2}$) system :

$$\Psi(t) = \begin{pmatrix} u(t) \\ v(t) \end{pmatrix}$$

TDSE has the form :
$$\begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \begin{pmatrix} u(t) \\ v(t) \end{pmatrix} = \begin{pmatrix} i\hbar \dot{u}(t) \\ i\hbar \dot{v}(t) \end{pmatrix}$$

An important class of solutions : **STATIONARY SOLUTIONS**

$$\begin{pmatrix} u(t) \\ v(t) \end{pmatrix} = \begin{pmatrix} u_0 e^{-iEt/\hbar} \\ v_0 e^{-iEt/\hbar} \end{pmatrix} = \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} e^{-iEt/\hbar}$$

Then SE becomes time-independent :

$$\begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} = E \begin{pmatrix} u_0 \\ v_0 \end{pmatrix}$$

Stationary states are determined by

an EIGENVALUE/EIGENVECTOR problem

7

* Spin- $\frac{1}{2}$ system : Hilbert space is 2-dimensional.

$$\psi = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \quad \text{[scribble]} \quad c_1, c_2 \text{ complex}$$

* Particle in 1D : $\psi(x)$

[scribble] Has an infinite # of ^{complex} components

One at every x .

Hilbert space is infinite-dimensional.

* Particle in 3D : [scribble] $\psi(\vec{r})$

One complex component at every \vec{r}

Hilbert space is ∞ -dimensional

* An INNER PRODUCT is defined in Hilbert space, analogous to dot product.

~~[scribble]~~

For a spin- $\frac{1}{2}$ system, if

$$\phi = \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}, \quad \psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}, \quad \text{then}$$

[scribble]

$$\langle \phi | \psi \rangle = \phi^\dagger \psi = (\phi_1^* \quad \phi_2^*) \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$$

$$= \phi_1^* \psi_1 + \phi_2^* \psi_2$$

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For ~~system~~ system with D -dimensional Hilbert space: if

$$\phi = \begin{pmatrix} \phi_1 \\ \vdots \\ \phi_D \end{pmatrix}$$

$$\psi = \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_D \end{pmatrix}$$

then

$$\langle \phi | \psi \rangle = \phi_1^* \psi_1 + \phi_2^* \psi_2 + \dots + \phi_D^* \psi_D$$

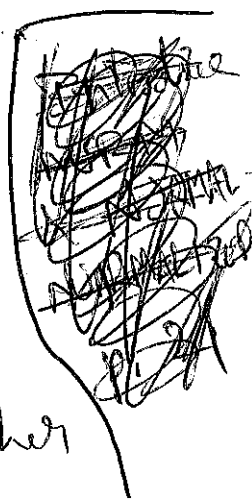
* For pde in 1 spatial dimension (infinite-dimensional Hilbert space)

~~Inner prod.~~ Inner prod. of $\phi(x)$ and $\psi(x)$

is

$$\int \phi^*(x) \psi(x) dx$$

* Inner product is called "overlap" of wavefunctions. When overlap = 0, the wavefunctions are ~~are~~ "orthogonal" to each other



* NORM and NORMALIZATION

For Euclidean vector, magnitude (norm) is square root of inner product with itself:

$$\vec{A} \cdot \vec{A} = A^2 \Rightarrow A = \sqrt{\vec{A} \cdot \vec{A}}$$

For wavevector, norm is (square root of inner product with itself): $N = \langle \psi | \psi \rangle$

~~•~~ ~~•~~ ~~•~~ The norm is \sqrt{N} .

Usually, we deal with wavevectors of unit norm:

$$\langle \psi | \psi \rangle = 1$$

Then the wavefunction is said to be ~~normalized~~

NORMALIZED

Multiplying a wavefunction by appropriate constant so that it becomes normalized \rightarrow NORMALIZING the wavefunction

9

A BRIEF HISTORY of QM

1900 (Planck): Light is emitted in quantized ~~lumps~~ lumps, having energy

$$E = hf = h\omega \quad [f \text{ or } \omega]$$

$$\omega = 2\pi f \quad \text{"angular frequency"}$$

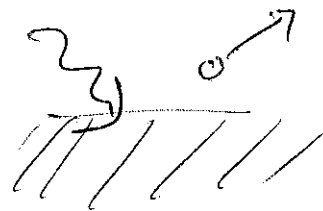
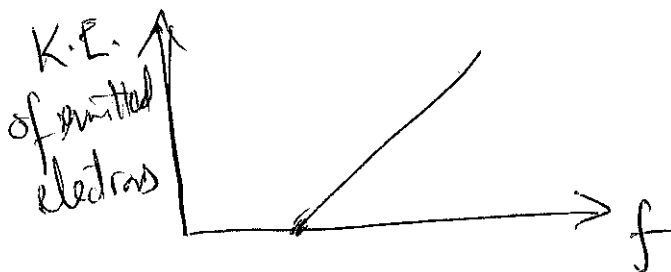
often called "frequency"

~~W~~
CORRECT
description
of BLACKBODY
RADIATION

[Note: for everyday purposes, the packets ("photons") are so small that light can be regarded as continuous]

1905 (Einstein): Light also propagates and is absorbed in ~~lumps~~ lumps. I.e., light is inherently quantized.

→ Explained the photoelectric effect.



For a light wave, $E = pc$

$E = hf = \frac{hc}{\lambda} \Rightarrow p = \frac{h}{\lambda}$

Momentum of photon.

Also $\frac{\omega}{c} = \frac{2\pi f}{c} = \frac{2\pi}{\lambda}$ is called

the wave number $k = \frac{\omega}{c} = \frac{2\pi}{\lambda}$

~~Photon momentum~~
Photon momentum

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

1913 (Bohr): Electrons in atoms have wavelike properties; hence ^{only} certain orbits are allowed... \Rightarrow "Explains" quantization of energy of atoms.

(Known from discrete atomic spectra.)

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1924 (de Broglie) All particles are associated with waves, with wavelength $\lambda = \frac{h}{p}$

"WAVE-PARTICLE DUALITY"

1925 (Heisenberg) Matrix formulation of QM

1925 (Schrödinger) Wave function formulation
[Schr. equation]

1926 (Born) Probabilistic interpretation

1926 (Dirac) Unification of viewpoints,
relativistic QM

~~INTERLUDE for p. (6)~~

~~One class of solutions: $\begin{pmatrix} \psi(t) \\ \chi(t) \end{pmatrix} = \begin{pmatrix} u \\ v \end{pmatrix} e^{-iEt/\hbar}$~~

~~Then SE becomes time-indep:~~

$$\begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = E \begin{pmatrix} u \\ v \end{pmatrix}$$

~~Stationary states determined by~~
~~An EIGENVALUE problem~~

* BLACK-BODY RADIATION

Feynman Lectures
Vol. 1, Ch. 41

(12)

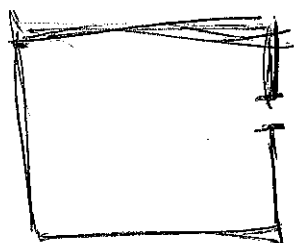
Vol. 3
Sec. 4-5

"Black body" → object that absorbs all ~~EM.~~ EM. waves (light etc.) incident on it.

→ An idealization. ~~...~~

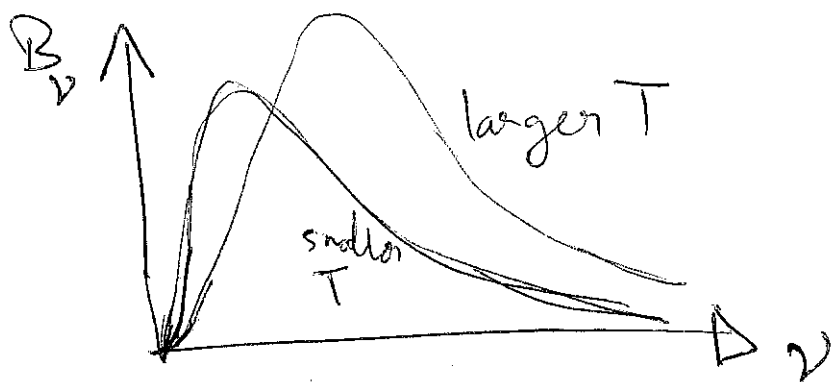
Experimental approximation: - black-coated surface,

- Better: large cavity with small aperture;



* When hot, emits EM. radiation, at all frequencies.

* Experiments performed, 19th century.



$B_\nu =$
spectral
radiance
per unit
frequency

* Theory of B_ν calculate # modes per unit frequency in cavity, ~~...~~

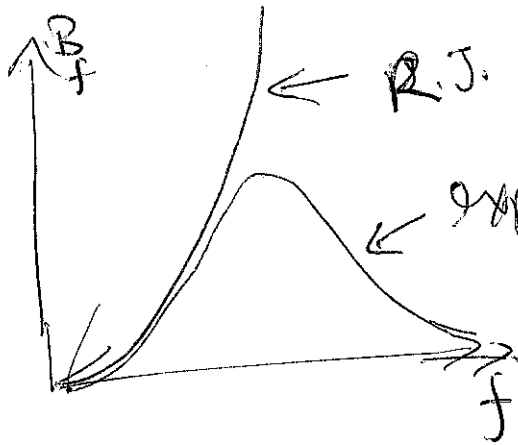
~~...~~ multiply by angle, c etc. factors and by ~~...~~ ENERGY PER MODE

WE
OMIT
these
steps

⑬ At temp. T , each mode carries energy?

Classical: $E = k_B T$ per mode.

\Rightarrow $B_f = \frac{2 k_B T}{c^2} f^2$ Rayleigh
Jeans
formulae



WRONG!

at large f ,

$B_f \rightarrow \infty$!

ULTRAVIOLET CATASTROPHE

* Correction to "mode per energy" required.

Classical: ~~probability~~ ~~distribⁿ~~ of energy!

$P(E) \propto e^{-E/k_B T}$ with E continuous

$\langle E \rangle = \frac{\int_0^\infty E e^{-E/k_B T}}{\int_0^\infty e^{-E/k_B T}} = k_B T$ SHOW

Quantum: $P(E) = e^{-nhf/k_B T}$ discrete

$\langle E \rangle = \frac{\sum_{n=0}^{\infty} e^{-nhf/k_B T} nhf}{\sum_{n=0}^{\infty} e^{-nhf/k_B T}} = \frac{hf}{e^{hf/k_B T} - 1}$

Use
 $\sum x^n = \frac{1}{1-x}$
 $\sum nx^n = \frac{x}{(1-x)^2}$

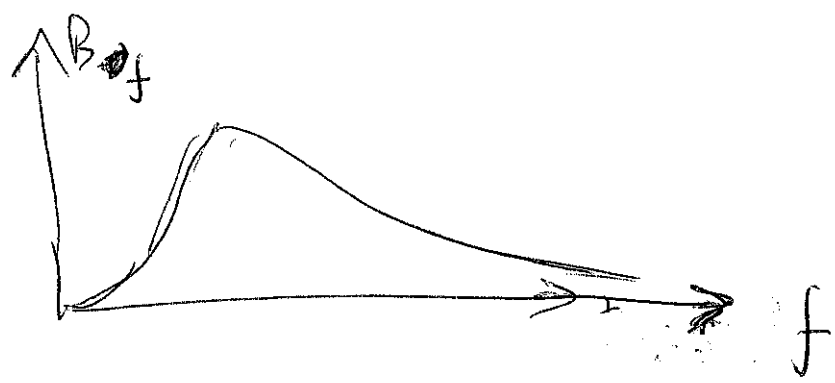
Replacing $k_B T \rightarrow \frac{h f}{e^{hf/k_B T} - 1}$ in R.J.

formula, Planck obtained the correct relation:

$$B_f = \frac{2 h^3}{c^2} \frac{f^3}{e^{hf/k_B T} - 1}$$

Planck distribution.

Matches expt.:



→ lesson: radiation in cavity/emitter exists in packets of energy $E = hf$.

~~* QUANTIZATION OF ENERGY~~

~~Observed in 19th energy:~~

~~Frequencies emitted by atoms are DISCRETE.~~

~~→ Fixed values for every atomic species~~

Feynman
Vol. III, Sec. 2-5

NOTE ON:

CONTINUOUS PROBABILITY DISTRIBUTIONS
VS. DISCRETE PROBABILITIES

14a

* Average of a continuous variable.

$y \in [a, b]$; probability $P(y)$; i.e. $\int_a^b P(y) dy = 1$

$$\text{Average (expectation value)} = \int_a^b dy y P(y)$$

if

Probability $\propto f(y)$? Have to normalise

first:
$$P(y) = \frac{f(y)}{\int_a^b dy f(y)}$$

So ~~\bar{y}~~
$$\bar{y} = \int dy y P(y) = \frac{\int dy y f(y)}{\int dy f(y)}$$

* Average of a discrete variable.

$m \in \mathbb{N}$, probabilities $P(m)$; $\sum_{m=1}^{\infty} P(m) = 1$

Average ~~\bar{m}~~
$$\bar{m} = \sum_{m=1}^{\infty} m P(m)$$

If Probability $\propto f_m$,

~~\bar{m}~~
$$\bar{m} = \frac{\sum_m m f_m}{\sum_m f_m}$$

* QUANTIZATION OF ENERGY

Feynman
Vol. III, Sec. 2-5

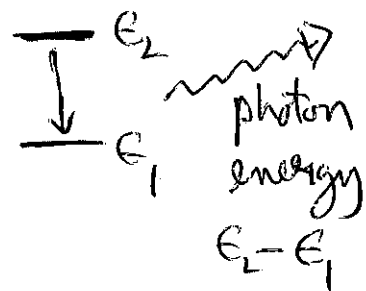
Observed in late 19th century:

- FREQUENCIES EMITTED BY ATOMS ARE DISCRETE
- FIXED VALUES for EVERY ATOMIC SPECIES

Quantum explanation:

① Energies of bound stationary states / orbits of electrons are DISCRETE. [Quantization of energy.]

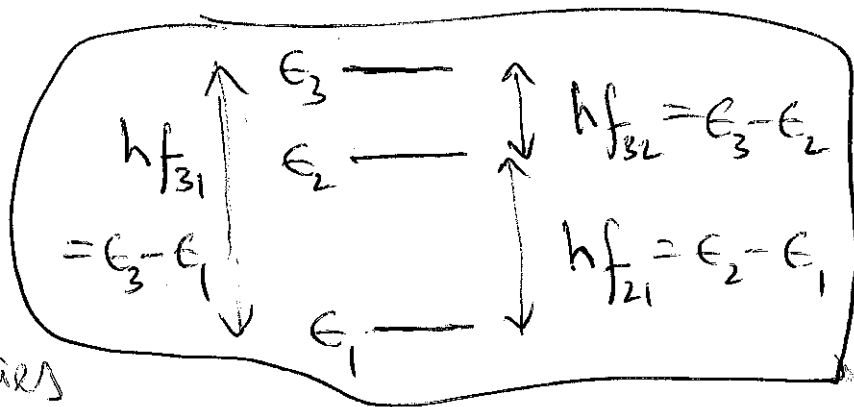
② Emission involves transition from higher → lower energy level.



③ Photon frequency $hf = E_2 - E_1$

An implication:

$$f_{31} = f_{32} + f_{21}$$



The discrete frequencies

in atomic spectra often come in triplets $\left\{ \begin{matrix} f_A, f_B, \\ f_A + f_B \end{matrix} \right\}$

→ Was noticed before QM. Explained by QM.

WHY SHOULD ENERGIES BE QUANTIZED?

de Broglie

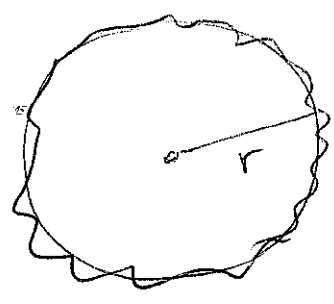
Quantization from the "wave" picture

① Orbits of an electron

Constructive interference

necessary for stationary

solution:



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

[de Broglie w. length $\lambda = \frac{h}{p}$]

⇒ only some radii are allowed

⇒ only some energies are allowed
($\frac{1}{2}mv^2$)

$$2\pi r = \frac{nh}{mv} \Rightarrow mvr = n \frac{h}{2\pi} = nh$$

Angular momentum $\Rightarrow L = mvr = nh$

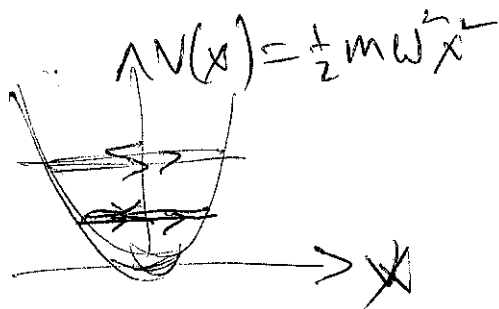
⇒ ~~this quantization~~ Bohr's model of the hydrogen atom is based on this quantization

~~condition~~ condition for angular momentum.



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② Harmonic oscillator ~~Quantum harmonic oscillator~~

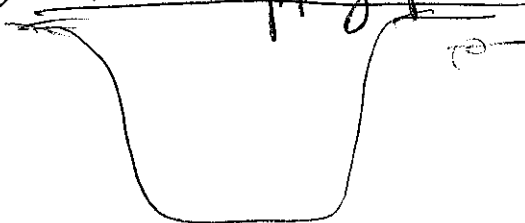


Constructive interference only
for some path lengths \Rightarrow
only for some energies.

Energies turn out to be $E_n = (n + \frac{1}{2}) \hbar \omega$

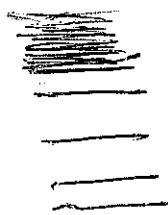
ω is sometimes called the "trapping frequency"

③ Other trapping potential



Energies of bound states
are discrete

Energies of non-bound states ("scattering" states)
are continuous (all energies possible)



For non-bound states, no "interference".

* Quantization from the SE

~~Stationary~~ Stationary solutions are given by

eigenvalue equations $H\psi = E\psi$

For finite-dimensional Hilbert spaces,

$$\left(H \right) \left(\psi \right) = E \left(\psi \right)$$

only D eigenvalues for D -dimensional problem

\Rightarrow obviously discrete energies.

For ~~infinite~~ ∞ -dim. Hilbert spaces, e.g., a

pde in 3D: $\left[-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}) \right] \psi(\vec{r}) = E \psi(\vec{r})$

also an eigenvalue problem, with infinite

of solutions. E can be discrete or

continuous. E.g., for $V(\vec{r}) = 0$, the

~~allowed~~ allowed energy values are continuous.

For $V(\vec{r}) = \frac{1}{2} m \omega^2 (x^2 + y^2 + z^2)$, the energies

are discrete.

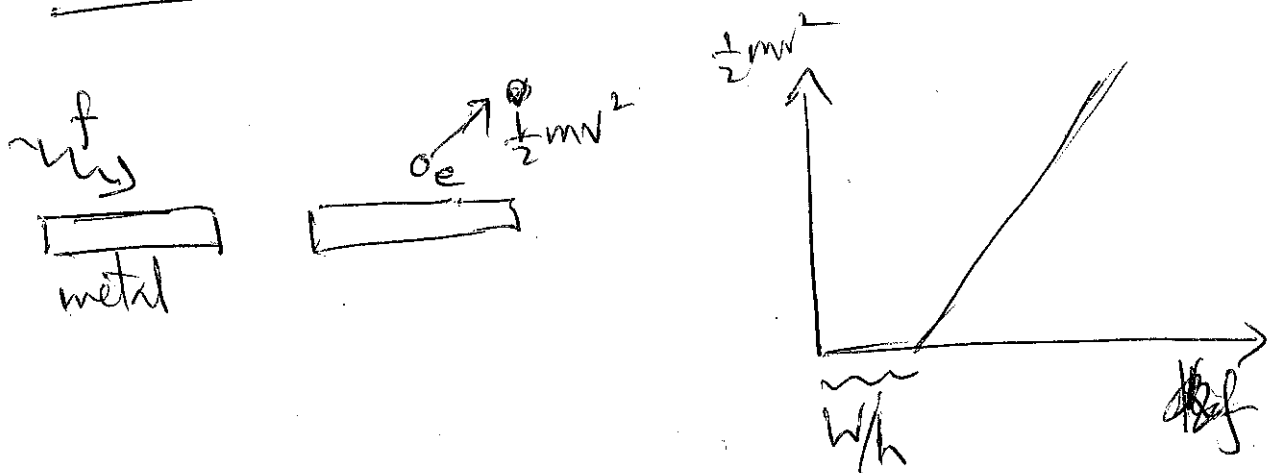
In 1D: $V(x) = 0$ continuous spectrum

$$E = \frac{\hbar^2 k^2}{2m}$$

$V(x) = \frac{1}{2} m \omega^2 x^2$ discrete spectrum $E_n = (n + \frac{1}{2}) \hbar \omega$

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* THE PHOTOELECTRIC EFFECT



Why this behavior?

If electron receives energy E from light,

$$\frac{1}{2}mv^2 = E - W$$

W = energy required to overcome binding to metal. ("work function")

New idea (Einstein 1905): energy

$E = hf$, light comes in packets (photons):

$$\frac{1}{2}mv^2 = hf - W$$

Linear dependence with frequency!

Experimental behavior explained using photon picture.