

INTRODUCTION TO QUANTUM MECHANICS

PART- I The TRANSITION from CLASSICAL to QUANTUM PHYSICS

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References

R. Eisberg and R. Resnick, "Quantum Physics," 2nd Edition, Wiley, 1985.
Chapters 1 and 3

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Volume I, Chapter 32 and Chapter 41 (Section 41-2, 41-3)

CHAPTER 3

THE ORIGINS OF QUANTUM PHYSICS

- By the end of the 19th century, classical physics appeared to be on solid foundations. The universe was conceived as containing matter consisting of
 - particles**, obeying Newton's law of motion;
 - and
 - radiation (waves)** obeying Maxwell's equation of electromagnetism.Einstein's theory of special relativity generalized classical physics to include the region of high velocities.

- Some key experiments, however, could not be explained by classical physics,
 - Blackbody Radiation
 - Photoelectric Effect
 - Compton Effectwhich forced the introduction of radical new concepts:
 - Quantization of physical quantities
 - Particle properties of radiation
 - Wave properties of particles

In the previous chapter we reviewed the strength of classical physics (electromagnetism and relativity.) In this chapter we aim to familiarize with the topics that forced a transition from classical to quantum concepts.

3.1 BLACKBODY RADIATION¹

On December 14, 1900, at a meeting of the German Physical Society, Max Planck presented his paper "On the Theory of the Energy Distribution Law of the Normal Spectrum." This date is considered to be **the birthday of quantum physics**. He broke ranks with the then quite accepted "law of equipartition energy" that stated that the average energy of, for example, a harmonic oscillator was independent of its natural frequency. He instead postulated a frequency-dependent average energy and, very revolutionary, that

the energy could have only discrete (quantized) values. Planck presented his paper while trying to explain the observed properties of thermal radiation. In this section we will review that development, as to gain some grasp of why the discreteness of a physical property lead to a radical different behavior of matter.

The problem that Plank had at hand was related to thermal radiation. Thermal radiation refers to the emission of electromagnetic waves by any object at a given temperature absolute temperature T . Matter in a condensed state (solid or liquid) emits a continuous spectrum of radiation. But even at temperatures as high as a few thousand of degrees Kelvin, most of the radiation is invisible to us as they lie in the infrared part of the electromagnetic spectrum.

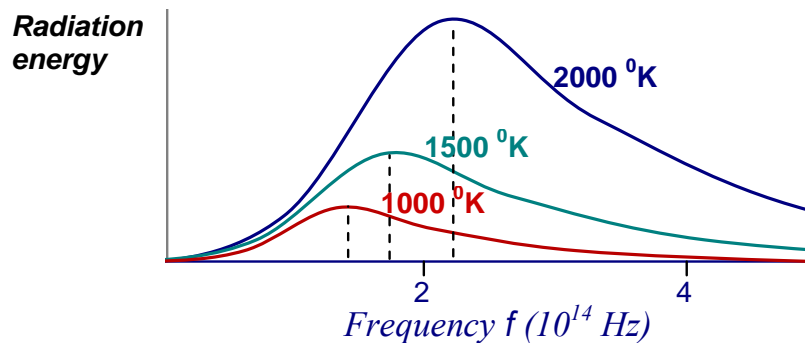


Fig 3.1 Spectral thermal radiance of a body showing the strong dependence on the body's temperatures.

With increasing temperature the body emits more radiation while the frequency of the most intense radiation (see dashed lines) also increases. The relationship between the temperature of a body and the frequency spectrum allows estimating the temperature of a hot body, such as a star, by observing the radiation it emits.

The detailed form of the spectrum depends somewhat upon the composition of the body. HOWEVER, there exist a type of body configuration that emit thermal spectra of a **universal character**. These are called blackbodies (they efficiently absorb all radiation incident upon them.) Independent of the details of their composition, it is found that

all blackbodies at the same temperature emit thermal radiation with the same spectrum (1)

It turns out that,

- while the invariability of the spectrum from blackbody to blackbody can be explained based on thermodynamic arguments (see **Kirchoff's law** below, which states that the ratio of the emissive power \mathcal{P}_e to the absorption coefficient a is the same for all bodies at the same temperature.)
- the specific form of the spectrum (tending to zero at very low and very high frequencies) can not be explained in terms of classical physics arguments. (**Planck** was able to solve this problem on the basis of quantum arguments.)

Section 3.1 describes in more detail these two aspects.

3.1.A The Kirchoff' Law and the Concept of Blackbody Radiator

3.1.A.a Macro-scale heat-transfer concepts

Heat transfer

While heat transfer Q by conduction and convection requires a material medium, radiation does not.

Thermal Radiation

Refers to the emission of electromagnetic waves by any object at a given temperature absolute temperature T .

Experimentally it was found (in 1879) that the rate at which a system emits radiation is proportional to the fourth power of *its* absolute temperature

$$\frac{\Delta Q}{\Delta t} \sim T_{object}^4$$

Since the rate of radiative heat flow is also proportional to the area of the object, the emitted power per unit area is typically expressed as,

$$R_{emitted} = \frac{1}{A} \frac{\Delta Q}{\Delta t} = e \sigma T_{object}^4 \quad (2)$$

$\sigma = 5.67 \times 10^{-8} \text{ W/m}^2 \cdot \text{K}^4$
 Stefan-Boltzman constant
 Emissivity of the surface ($0 < e < 1$)

Absorbed Radiation

A system absorbs radiation proportional to the fourth power of the absolute temperature of its *surroundings*.

$$R_{absorbed} = a \sigma T_{surrounding}^4 \quad (3)$$

“a” indicates the relative ability of the
 surface to absorb radiation ($0 < a < 1$)

For an object in equilibrium with its surrounding:

$$R_{emitted} = R_{absorbed} , \text{ which implies } e = a \quad (4)$$

That is,

Good radiators (e) are good absorbers (a)

Heat flow via radiation from an object of area A to its surroundings

$$\frac{\Delta Q}{\Delta t} = e A \sigma (T_{object}^4 - T_{surroundings}^4) \quad (5)$$

3.1.A.b Kirchhoff's law

The emissive power \mathcal{P}_e of a given material is defined as follows (see also Fig. 3.2A for identifying the variables being used)

$\mathcal{P}_e(\vec{k}) d\omega d\Omega =$ emitted power per unit area of the body,
 composed of electromagnetic radiation of
 frequency between ω and $\omega+d\omega$, and
 directed into a solid angle $d\Omega$ about the
 direction \vec{k}

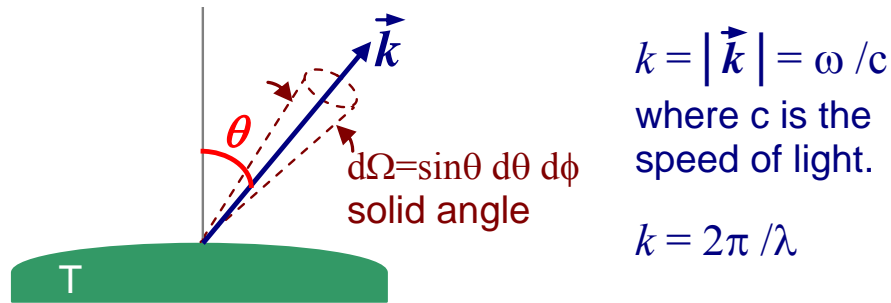


Fig. 3.2A Radiation of wave-vector around \mathbf{k} emitted by a surface at temperature T .

G. R. Kirchhoff proved in 1859 by using general thermodynamic arguments that, at any given electromagnetic wavelength,
the ratio of the emissive power \mathcal{P}_e to the absorption coefficient a is the same for all bodies at the same temperature

$$\left. \frac{\mathcal{P}_e}{a} \right|_1 = \left. \frac{\mathcal{P}_e}{a} \right|_2 = \left. \frac{\mathcal{P}_e}{a} \right|_3 = \text{etc} \quad (6)$$

Blackbody Radiator

*A perfect radiator would have an absorption Coefficient $a=1$
 Such a system is called a blackbody radiator* (7)

Note: The “blackbody” name originates from the fact that “black looking” objects are in fact objects that do not reflect any of the incident light. “Black color” is in fact an absence of color.

BUT in the context of the quantum physics that we are developing here, a blackbody radiator may not appear black at all. In fact, a blackbody emits very efficiently all colors.

3.1.A.c Cavity's aperture as an approximation to a blackbody radiator

A blackbody radiator is an idealization; however, a small orifice in a cavity closely approximates one.

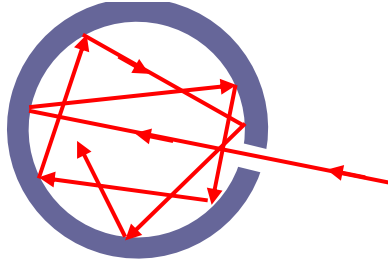


Fig. 3.2B Blackbody radiator.

- Any radiation incident from the outside and passing through the hole will almost completely be absorbed in multiple reflections inside the cavity; that is, the hole has an effective absorption coefficient close to unity ($a=1$)
- Since the cavity is in thermal equilibrium, the radiation getting inside through the small opening and that escaping from the small opening will be equal ($e=1$). We infer that the spectral characteristics of the radiation emitted by the aperture should have then the characteristics of a blackbody radiator.

3.1.B Radiation in a cavity

- Our next objective is to characterize the bath of electromagnetic radiation existent inside a blackbody radiator cavity. We would like to know,

How much light energy of angular frequency ω (across the electromagnetic spectrum) does exist inside the cavity at equilibrium conditions at a given temperature T ? (8)

Two approaches for answering this question, each arriving to the same general result, are worth mentioning:

APPROACH -1: The first follows a Feynman's description (very rich in physics content) that models an atom as an electrical harmonic oscillator. The equilibrium inside the cavity is obtained by a balance between:

- the energy absorbed by the atom from the light energy existent in the cavity, and

- the amount of energy that the atom scatters out (since accelerated charges emit radiation.)

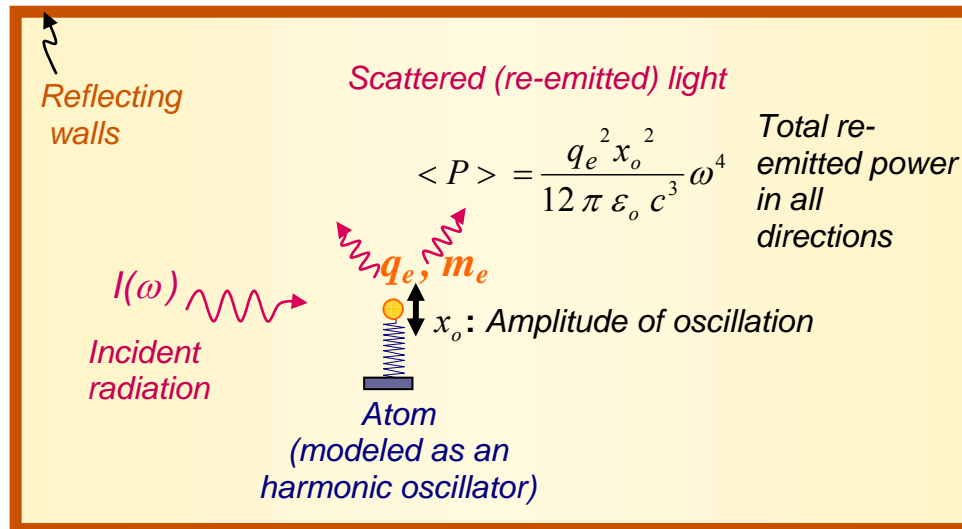


Fig. 3.3 Atom in equilibrium with a bath of electromagnetic radiation inside a box a perfectly reflecting walls.

By equating a) the rate of energy absorption by the atom (which depends on the intensity of radiation $I(\omega)$) and b) the rate of energy emission (given by $\langle P \rangle$), an analytical expression will be obtained for the required *Light Intensity Spectral Density* $I(\omega)$ that must exist inside the cavity (for an equilibrium situation to prevail.)

(Comment: Since the incident radiation $I(\omega)$ is made out of electromagnetic fields, it is plausible to relate it to the amplitude of oscillation x_o . That is, the greater the light intensity, the larger the charge's amplitude of oscillation, and thus the greater $\langle P \rangle$, which, apparently, would lead to no restriction on the particular value that $I(\omega)$ should take. However, the peculiar dependence of $\langle P \rangle$ on ω (which is dictated by the physics laws) adds an additional constrain on $I(\omega)$. For a given frequency ω , $I(\omega)$ can not be not too big nor too small, but the right amount as to make the energy balance to prevail.)

APPROACH-2: The second approach is a bit more abstract; it considers the energy-interchange equilibrium reached between

the electromagnetic-modes inside the cavity and the cavity's walls. It involves the counting of electromagnetic modes. An expression for the Light Energy Density $U(\omega)$ at equilibrium will be obtained.

The consistency of these two views will be verified through the relationship $I(\omega) = c U(\omega)$ where c is the speed of light.

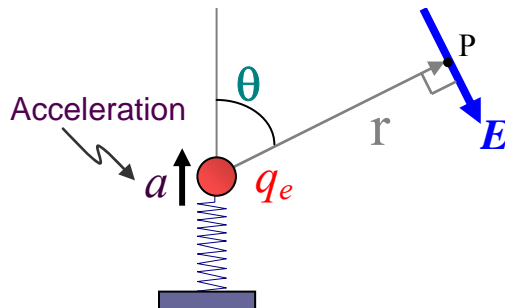
- It turns out that the procedure followed by these two approaches (leading to an expression for $I(\omega)$ and $U(\omega)$ respectively) have survived the new wave of quantum concepts; that is, they are still considered valid. **What has changed then?**

What has changed dramatically, due to the advent of the quantum ideas, is the specific way to calculate the average-energy of an atom (in approach-1 method) or the average energy of an electromagnetic mode (approach-2 method.) A detailed description of these quantum modifications incurred in the calculation of $I(\omega)$ and $U(\omega)$ constitutes the essence of Chapter 3.

- In what follows, we will mainly concentrate on a detailed account of the approach-1 referred above. A description of the approach-2 is given in the appendix.

3.1.B.a Emission of radiation by an accelerated charge²

Electromagnetic radiation is emitted by charges in accelerated motion.



Electric field E produced by an accelerated charge. At a point “P”, E is oriented perpendicular to the line of sight and its magnitude proportional to the component of the acceleration-vector along the direction perpendicular to the line of sight.

Fig. 3.4 An electron in an atom modeled as a charge attached to the end of a spring of appropriate spring constant of natural frequency ω_o .

$$E(r, t) = \frac{-q_e \sin(\theta)}{4\pi\epsilon_o c^2} \frac{1}{r} a(t - \underbrace{r/c}_{\text{Retardation time}}) \quad \text{Electric field produced by an accelerated charge } q_e \quad (9)$$

The Poynting vector \vec{S}

$$\vec{S} = \epsilon_o E^2 \vec{c} \quad \text{Its magnitude } S \text{ gives the amount of energy per square meter per unit time that passes through a surface that is normal to the direction of propagation.} \quad (10)$$

Radiation power P emitted by an accelerated charge

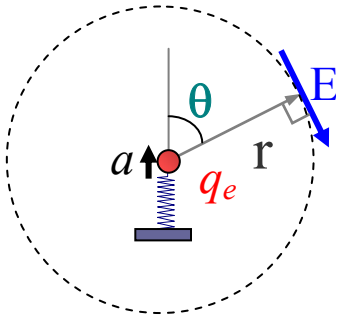


Fig. 3.5 Electromagnetic power radiated by an accelerated charge.

$$\begin{aligned} P &= \int S \, dA = \\ &\quad \text{Integral over a sphere of radius } r \\ &= \int \left[\epsilon_o c \frac{q_e^2 \sin^2(\theta)}{(4\pi\epsilon_o c^2)^2} \frac{1}{r^2} a'^2 \right] dA \\ P &= \frac{q_e^2}{6\pi\epsilon_o c^3} a'^2 \quad (11) \\ \text{where } a' &\equiv a(t') = a(t - r/c) \end{aligned}$$

Emission of radiation by a charge under harmonic oscillation

Consider that a charge q_e oscillates with angular frequency ω

$$x(t) = \text{Real} \left\{ \underbrace{x_o e^{j\omega t}}_{\text{Complex variable}} \right\} = x_o \cos(\omega t) \quad (12)$$

Here, ω is not necessarily the natural frequency ω_0 of the oscillator (see Fig 3.8). For example, the oscillator may be being driven by a external source of arbitrary frequency ω .

In what follows we will be evaluating time averages of physical quantities (let's call it g) over one period $T = 2\pi / \omega$ of oscillation:

$$\langle g \rangle = \frac{1}{T} \int_0^T g(t) dt \quad (13)$$

Notice, for example, that the time average of $\cos^2(\omega t)$ over one period is $1/2$.

We also will be using indistinctly $\cos(\omega t)$ or $e^{j\omega t}$. For the latter it is assume that we will take the real part after the calculations in order to obtain a proper (classical) physical interpretation.

From expression (11) we calculate an acceleration $a' = -\omega^2 x_o e^{j\omega t}$

and $\langle a'^2 \rangle = (1/2) \omega^4 |x_o|^2$. Replacing these values in expression (11) gives,

$$\langle P \rangle = \frac{q_e^2 |x_o|^2}{12\pi\epsilon_o c^3} \omega^4 \quad \text{Total average power emitted by a charge } q_e \text{ undergoing harmonic oscillations with amplitude } x_o, \text{ and angular frequency } \omega. \quad (14)$$

3.1.B.b Light Scattering

Consider a plane wave (filling all the space) traveling in a specific direction, let's say +X. Here we highlight only the temporal variation:

$$E(t) = \text{Real} \{ E_o e^{j\omega t} \} = E_o \cos(\omega t) \quad (15)$$

time variation of the electric field of the incident radiation.

A traveling wave carries energy. A quantification of this travelling energy is expressed by the corresponding Poynting vector $\vec{S} = \epsilon_o E^2 \vec{c}$; its average value, according to (12), is equal to,

$$\langle S \rangle = \frac{1}{2} \epsilon_o c E_o^2 \quad (16)$$

$\langle S \rangle$ is the average energy per square meter per unit time passing through a surface normal to the direction of propagation.

$$\langle S \rangle = \frac{1}{2} \epsilon_0 c E_o^2$$

$\langle S \rangle$ is also called the intensity "I"

E_o is the amplitude of the electric field of the incident wave

$E = E_o e^{j\omega t}$

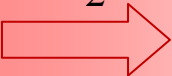


Fig. 3.6 Incident plane-wave radiation of frequency ω .

When an atom characterized by a resonance frequency ω_o , is placed in a region where there is a bath of electromagnetic radiation, the radiation's electric field $E = E_o e^{j\omega t}$ will drive the atom's charge q_e up and down; that is, it will accelerate the charge thus causing the atom to re-emit electromagnetic radiation. This process is called **scattering**. That is,

scattering is the process by which energy is absorbed by an atom from the incident radiation field and re-emitted in all directions. (17)

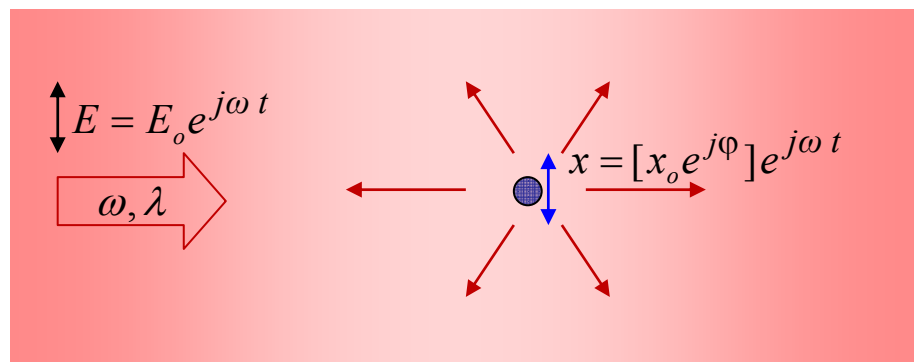


Fig. 3.7 Incident light is absorbed and (re-emitted) scattered by an atom in all directions.

Let's calculate the energy absorbed (hence re-emitted) by the charge

Actually the energy emitted by the accelerated charge has already been calculated in expression (14) above, except that we need to find out the amplitude of oscillation x_o ; the latter will depend on the electric field amplitude E_o , as well as the frequency ω of the incident radiation. In other words, let's calculate the relationship between E_o , ω , and x_o .

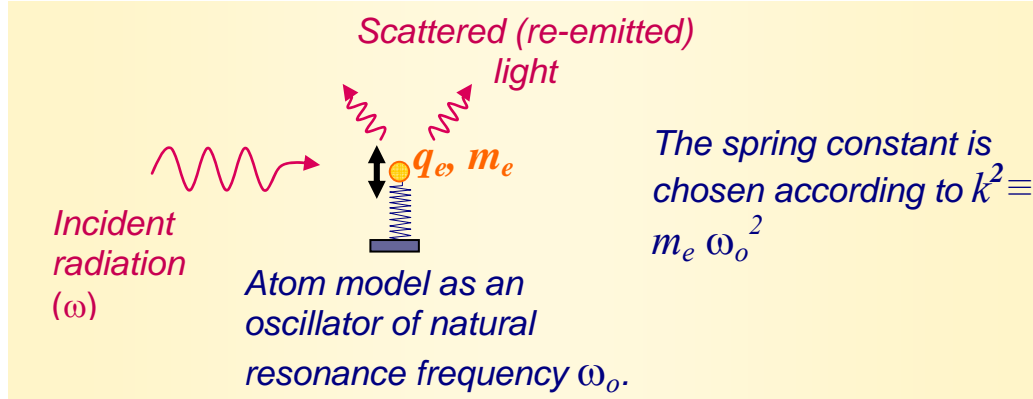


Fig. 3.8 Atom modeled as an oscillator of natural frequency ω_o . The ability of the oscillator to absorb energy from the incident radiation depends on ω .

To find x_o , let's model the atom as a damped harmonic oscillator. Accordingly the equation of motion for the charge q_e is given by,

$$m_e \frac{d^2 x}{dt^2} + m_e \gamma \frac{dx}{dt} + kx = q_e E_o e^{j\omega t} \quad (18)$$

Here the term $m_e \gamma \frac{dx}{dt}$ accounts for the presence of a dissipation energy source, which, in our case, can be identified in the loss of energy due to the electromagnetic radiation by the accelerated charge.

A stationary solution of (18) is given by,

$$x = [x_o e^{j\varphi}] e^{j\omega t} \quad (19)$$

where

$$x_o = x_o(\omega) = \frac{(q_e / m_e) E_o}{\left[(\omega_o^2 - \omega^2)^2 + \gamma^2 \omega^2 \right]^{1/2}} \quad \text{Amplitude of oscillation as a function of frequency} \quad (20)$$

and

$$\phi = \tan^{-1} \left(- \frac{\gamma \omega}{\omega_o^2 - \omega^2} \right) \quad (20)'$$

Expression (20) indicates that the amplitude of oscillation x_o (and hence the acceleration) of the charge depends on the incident radiation's frequency ω .

Let's proceed now to calculate the total power radiate by the accelerated charge under the influence of an electric filed of amplitude E_o and frequency ω . Replacing the value of x_o given in (20)

for x_o into the expression for the radiation power $\langle P \rangle = \frac{q_e^2 x_o^2}{12\pi\epsilon_o c^3} \omega^4$

given in (14), one obtains, $\langle P \rangle = \frac{q_e^2}{12\pi\epsilon_o c^3} \omega^4 \frac{(q_e / m_e)^2 E_o^2}{(\omega_o^2 - \omega^2)^2 + (\gamma \omega)^2}$.

Rearranging terms,

$$\langle P \rangle = \left[\frac{1}{2} \epsilon_o c E_o^2 \right] \frac{8\pi}{3} \left(\frac{q_e^2}{4\pi\epsilon_o m_e c^2} \right)^2 \frac{\omega^4}{(\omega_o^2 - \omega^2)^2 + (\gamma \omega)^2} \quad (21)$$

Expression (21) gives the total average energy emitted by the charge q_e when subjected to a harmonic electric field (given in expression (15))of amplitude E_o and frequency ω .

The concept of scattering cross section

If we considered a hypothetical cross section of area σ intersecting the incident radiation, the amount of energy per second hitting that area would be

$$\langle P \rangle = \left[\frac{1}{2} \epsilon_o c E_o^2 \right] \sigma = I \sigma \quad (22)$$

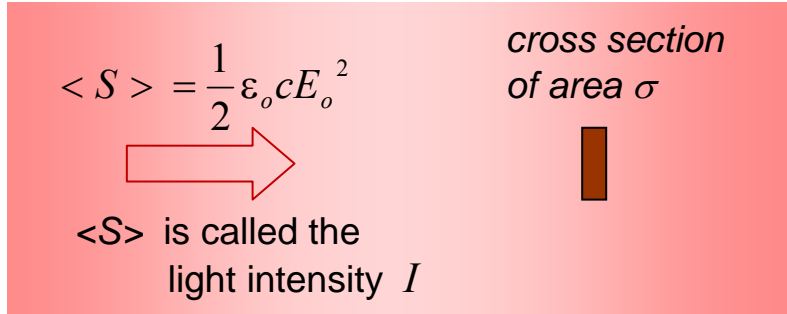


Fig. 3.9 Pictorial representation of scattering cross section.

One can use the analogy of an effective area being intercepted by the incident radiation to define how effectively the radiation is absorbed and scattered (*i. e.* re-emitted) by an atom. In effect, comparing expressions (21) and (22), the total power scattered by an atom is numerically equal to the energy per second incident on a “surface” of cross-section area $\sigma_{\text{scattering}}$,

$$\langle P \rangle_{\text{scattering}} = \left[\frac{1}{2} \epsilon_o c E_o^2 \right] \sigma_{\text{scattering}} \quad (23)$$

where

$$\sigma_{\text{scattering}} = \frac{8\pi}{3} \left(\frac{q_e^2}{4\pi\epsilon_o m_e c^2} \right)^2 \frac{\omega^4}{(\omega_o^2 - \omega^2)^2 + (\gamma\omega)^2} \quad (24)$$

$\sigma_{\text{scattering}}$ has units of area.

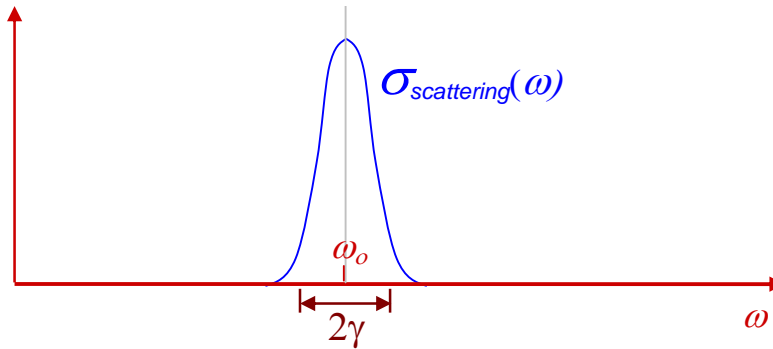


Fig. 3.10 Sketch of the atom's scattering cross section.

Certainly, every photon absorbed by the atom will be scattered out. But what expression (24) is suggesting is that photons of frequency ω quite different than ω_o will have little chance to be absorbed (and re-emitted.) The closer ω is to ω_o , the higher the chances to be absorbed (and subsequently be re-emitted.)

3.1.B.c Electromagnetic Radiation Damping

We address here the fact that

the term $m_e \gamma \frac{dx}{dt}$ in Eq. (18) (the term in the differential equation that takes into account the energy dissipation,) should be compatible with expression (21) (that gives the electromagnetic energy dissipated by the oscillator.)

We should require then that these two expressions be consistent with each other.

Indeed,

- on one hand, the power dissipated by an oscillator is given by

$$[force] \times (velocity) = [m_e \gamma \frac{dx}{dt}] (\frac{dx}{dt}) = [m_e \gamma (j\omega x)] (j\omega x) = -m_e \gamma \omega^2 x^2.$$

Here we use the expression for $x(t)$ given in (19) $x = [x_o e^{j\varphi}] e^{j\omega t}$.

The average value of the dissipated power will be,

$$-(1/2)m_e \gamma \omega^2 x_o^2.$$

- On the other hand, according to (14), the emitted electromagnetic power is,

$$\langle P \rangle = \frac{q^2 x_o^2}{12\pi\epsilon_o c^3} \omega^4$$

The last two expressions should be equal.

$$(1/2)m_e \gamma \omega^2 x_o^2 = \frac{q^2 x_o^2}{12\pi\epsilon_o c^3} \omega^4$$

This allows to identify $\gamma = \frac{q^2}{6\pi\epsilon_o m_e c^3} \omega^2$. Rearranging terms,

$$\gamma = \frac{2}{3c} \frac{q_e^2}{4\pi\epsilon_o m_e c^2} \omega^2 \quad \text{electromagnetic radiation damping constant} \quad (25)$$

For practical purposes, however (given the very narrow bandwidth of the cross section $\sigma(\omega)$ shown in Fig 3.10 above,) γ will be typically end up being evaluated at $\omega = \omega_0$, (i.e. the narrow bandwidth of $\sigma(\omega)$ tell us that most of the physics happens around $\omega = \omega_0$.)

Rate at which the oscillator loses energy

(A more detailed description of this section is given in the supplementary Appendix-3 of this chapter.)

Let

$$W = W(t) \quad \text{be the average energy of an oscillating charge at a given time } t. \quad (26)$$

If the oscillating charge is left alone to oscillate, its amplitude of vibration will die out progressively as the oscillator loses its mechanical energy by emitting electromagnetic radiation.

The rate at which the oscillating charge loses energy is given by,

$$\frac{dW}{dt} = -\gamma W \quad (27)$$

with its corresponding solution

$$W(t) = W_0 e^{-\gamma t} \quad (28)$$

As an example, an atom that has a resonance frequency corresponding to $\lambda = 600 \text{ nm}$, would have a damping constant of $\gamma \sim 10^8 \text{ s}^{-1}$. That is, the radiation will effectively die out after $\sim 10^{-8} \text{ s}$ (or after $\sim 10^7$ oscillations.)

3.1.C Radiation and thermal equilibrium

Let's consider an atom enclosed in a box made of mirror walls which contains electromagnetic radiation. Radiation re-emitted by the atom remains inside the box undergoing multiple bounces on the mirror walls. Let's further assume that the *temperature* of the whole system is T .

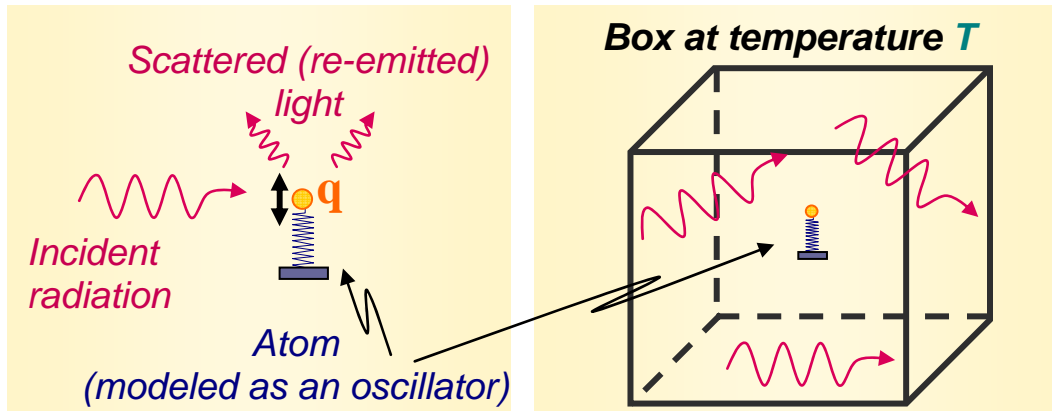


Fig. 3.10 Schematic representation of an atom as an harmonic oscillator that radiates energy. The atoms absorb energy from the electromagnetic radiation existent inside the box (the latter assumed to be made of perfectly reflecting walls.)

How to make the temperature T intervene in an expression like (14) that gives the power scattered by an atom in the form

$$\langle P \rangle_{\text{scattering}} = \frac{q_e^2 |x_o|^2}{12\pi\epsilon_o c^3} \omega^4 ?$$

It is plausible to assume that the equilibrium temperature should correspond to proper value of the amplitude of the electric field, E_o , since the higher the value of E_o , the higher the charge's amplitude of vibration x_o , the greater temperature to be associated with the atom (i.e. the amplitude of the oscillator should increase with temperature.)

If our assumption were correct, how to find then the proper value of E_o corresponding to a given temperature T ?

Aiming to find a proper answer let's outline some considerations:

- If an atomic oscillator had no charge, it would oscillate forever. It would have an average energy W compatible with the temperature in the box; that is $W = W(T)$. In other words, it would oscillate forever with an amplitude settled by the temperature T in the box. $\frac{1}{2} k x_o^2 = \frac{1}{2} kT$ or $\frac{1}{2} m \omega_o^2 x_o^2 = \frac{1}{2} kT$.
- But our atomic oscillator is charged. If it were left alone, its amplitude of vibration x_o would die out progressively, as the oscillator loses its energy by emitting electromagnetic radiation.

- If our atomic charged oscillator were in physical contact with other atoms, energy in the proper amount will be supplied by their mutual collisions as to keep the same temperature among themselves.

Here, however, we will consider that the energy is supplied via electromagnetic interaction: the atom draws energy from the radiation existent in the cavity to compensate the energy being lost by radiation (accelerated charged particles emit radiation.) When this compensation of energy matches, then we are at an equilibrium situation, which inherently should occur at a given temperature (the latter settling the charge's amplitude of oscillation at a corresponding value.) We will retake the subject of temperature dependence of x_0 in Section 3.1.c.b below.

3.1.C.a Light intensity spectral density $I(\omega)$ at equilibrium

To formalize the equilibrium situation we have to keep in mind that radiation of different frequencies might be present in the cavity. It is convenient, then, to introduce the concept of spectral density $I(\omega)$:

$I(\omega)$ = light intensity spectral density

$I(\omega) d\omega$ = light intensity of frequency ω within a range $(\omega, \omega + d\omega)$ inside the box

= contribution to the average electromagnetic energy per square meter per unit time passing through a surface normal to the direction of propagation from radiation components of frequency ω within a range $d\omega$

$$\text{Units of } [I(\omega)] = \frac{[\text{Intensity}]}{[\Delta\omega]} = \frac{J/(m^2s)}{1/s} = \frac{J}{m^2}$$

Before establishing the condition of equilibrium, let's make two pertinent observations:

- According to (21) and (22) (and keeping in mind that different frequencies ω can be present in the cavity) the total power emitted by the atom is given by $\int_0^\infty I(\omega)\sigma(\omega)d\omega$. But, in a scattering process, every photon incident is re-radiated by the atom of natural frequency ω_0 . (i. e. photon-in \rightarrow

photon-out.) Therefore the expression above can be interpreted as the rate at which energy is incident (and captured) by the atom.

- On the other hand, this same emission of power (i. e. $\int_0^\infty I(\omega)\sigma(\omega)d\omega$), can be seen from the perspective of a system loosing energy due to a damping process $\frac{d[W(\omega)]}{dt} = -\gamma(\omega)[W(\omega)]$ characterized by a damping constant $\gamma(\omega)$. Also, the requirement of compatibility between i) power re-radiated by the atom, and ii) a simple damping harmonic oscillator model $m_e \frac{d^2x}{dt^2} + m_e \gamma \frac{dx}{dt} + kx = q_e E_o e^{j\omega t}$, lead to expression (25) $\gamma(\omega) = \frac{2}{3c} \frac{q_e^2}{4\pi\epsilon_o m_e c^2} \omega^2$. But since all the dynamics occurs at $\omega=\omega_0$, that is $W(\omega) \sim 0$ for $\omega \neq \omega_0$, we can use $\frac{dW}{dt} = -\gamma(\omega_o) W$, with the interpretation that W is the total energy of the atom.

Formalization of the thermal equilibrium condition:

How much **light intensity spectral density** $I(\omega)$ there must be inside the box at temperature T for,

- the energy absorbed by the oscillator from the radiation bath per unit time

$$\frac{dW}{dt} = \int_0^\infty I(\omega)\sigma(\omega)d\omega \quad (29)$$

to be equal to

- the energy re-radiated by the oscillator per unit time

$$\frac{dW}{dt} = -\gamma \underbrace{W} \quad (30)$$

Average energy of the oscillator at temperature T

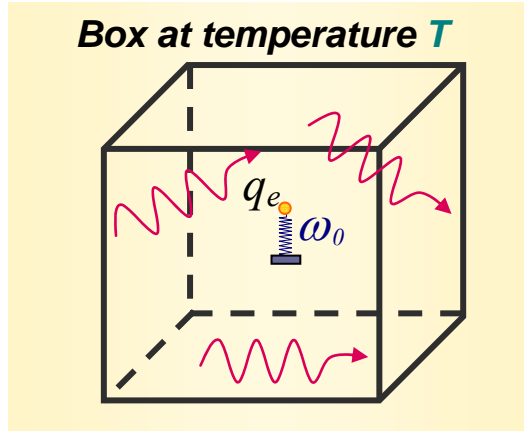


Fig. 3.11 Atom of natural frequency ω_0 in a bath of electromagnetic radiation of spectral density $I(\omega)$.

Let's evaluate the integral that appears in (29).

- Since the expression for $\sigma(\omega)$ peaks at $\omega \approx \omega_0$, then extending the integral down to $\omega = -\infty$ does not cause any significant change (this is done just to facilitate the calculation)

$$\int_0^\infty I(\omega)\sigma(\omega)d\omega = \int_{-\infty}^\infty I(\omega)\sigma(\omega)d\omega$$

$$\text{where } \sigma_{\text{scattering}} = \frac{8\pi}{3} \left(\frac{q_e^2}{4\pi\epsilon_0 m_e c^2} \right)^2 \frac{\omega^4}{(\omega_0^2 - \omega^2)^2 + (\gamma\omega)^2}$$

- For the same reason that only the values of ω very close to ω_0 will significantly contribute to the integral we can picture in our mind that

$$\int_{-\infty}^\infty I(\omega)\sigma(\omega)d\omega \approx \int_{\omega_0-\gamma}^{\omega_0+\gamma} I(\omega)\sigma(\omega)d\omega$$

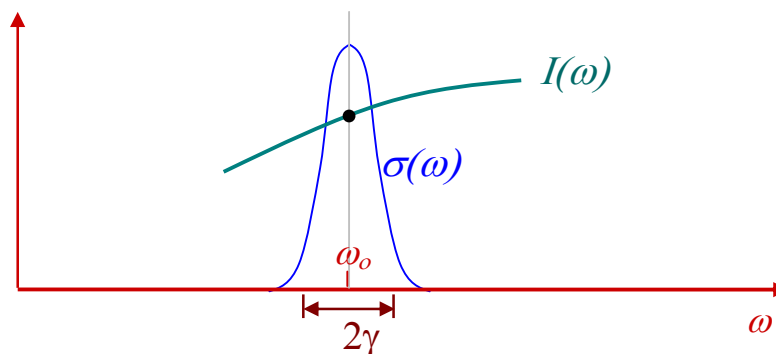


Fig.3.12 Sketch of the atom's scattering cross section and the spectral density light intensity present in side the cavity

Accordingly the following approximations can be considered appropriate,

$$\triangleright \omega^2 - \omega_o^2 = (\omega + \omega_o)(\omega - \omega_o) \approx (2\omega_o)(\omega - \omega_o)$$

$$\begin{aligned} \triangleright \frac{\omega^4}{(\omega_o^2 - \omega^2)^2 + (\gamma\omega)^2} &\approx \frac{\omega_o^4}{[\omega_o^2 - \omega^2]^2 + (\gamma\omega_o)^2} \\ &\approx \frac{\omega_o^4}{[(2\omega_o)(\omega - \omega_o)]^2 + (\gamma\omega_o)^2} \\ &\approx \frac{\omega_o^2}{4(\omega - \omega_o)^2 + \gamma^2} \end{aligned}$$

$$\triangleright I(\omega) \approx I(\omega_o)$$

All these approximations lead to

$$\begin{aligned} \int_0^\infty I(\omega)\sigma(\omega)d\omega &\approx \int_{-\infty}^\infty I(\omega)\sigma(\omega)d\omega \\ &= \int_{-\infty}^\infty I(\omega) \left[\frac{8\pi}{3} \left(\frac{q_e^2}{4\pi\epsilon_o m_e c^2} \right)^2 \frac{\omega^4}{(\omega_o^2 - \omega^2)^2 + (\gamma\omega)^2} \right] d\omega \\ &= \int_{-\infty}^\infty I(\omega) \left[\frac{8\pi}{3} \left(\frac{q_e^2}{4\pi\epsilon_o m_e c^2} \right)^2 \frac{\omega_o^2}{4(\omega - \omega_o)^2 + \gamma^2} \right] d\omega \\ &= I(\omega_o) \frac{2\pi}{3} \left(\frac{q_e^2}{4\pi\epsilon_o m_e c^2} \right)^2 \omega_o^2 \int_{-\infty}^\infty \left[\frac{1}{(\omega - \omega_o)^2 + (\gamma/2)^2} \right] d\omega \\ &\quad \left(\text{using } \int \frac{dx}{x^2 + a^2} = \frac{1}{a} \arctan \frac{x}{a} \right) \\ &= I(\omega_o) \frac{2\pi}{3} \left(\frac{q_e^2}{4\pi\epsilon_o m_e c^2} \right)^2 \omega_o^2 \frac{1}{\gamma/2} \left(\frac{\pi}{2} - \left(-\frac{\pi}{2}\right) \right) \\ &= I(\omega_o) \frac{2\pi}{3} \left(\frac{q_e^2}{4\pi\epsilon_o m_e c^2} \right)^2 \omega_o^2 \frac{2\pi}{\gamma} \end{aligned}$$

$$\int_0^\infty I(\omega)\sigma(\omega)d\omega = I(\omega_o) \frac{(2\pi)^2}{3\gamma} \left(\frac{q_e^2}{4\pi\epsilon_o m_e c^2} \right)^2 \omega_o^2 \quad (31)$$

At equilibrium we should have, $\frac{dW}{dt} = \int_0^\infty I(\omega)\sigma(\omega)d\omega = \left| \frac{dW}{dt} \right| = \gamma W$, which

leads to $I(\omega_o) \frac{(2\pi)^2}{3\gamma} \left(\frac{q_e^2}{4\pi\epsilon_o m_e c^2} \right)^2 \omega_o^2 = \gamma W$

$$I(\omega_o) = \frac{3}{(2\pi)^2} \left(\frac{4\pi\epsilon_o m_e c^2}{q_e^2} \right)^2 \frac{\gamma^2}{\omega_o^2} W$$

Using expression (25) for the value of $\gamma = \frac{2}{3c} \frac{q^2}{4\pi\epsilon_o m c^2} \omega^2$ evaluated

at $\omega = \omega_o$ one obtains, $I(\omega_o) = \frac{3}{(2\pi)^2} \left(\frac{4\pi\epsilon_o m_e c^2}{q_e^2} \right)^2 \left(\frac{2}{3c} \frac{q^2}{4\pi\epsilon_o m c^2} \right)^2 \omega_o^2 W$, or

$$I(\omega_o) = \frac{3}{(2\pi)^2} \left(\frac{2}{3c} \right)^2 \omega_o^2 W,$$

$$I(\omega_o) = \frac{1}{3\pi^2 c^2} \omega_o^2 \underbrace{W}_{\text{Average energy of the oscillator}} \quad (32)$$

$I(\omega_o)$ is the light spectral density at $\omega = \omega_o$.

Here ω_o is the natural frequency of the oscillator we were focusing in. Had we used an oscillator of a different natural frequency, let's say ω_o' , we would have obtained a similar expression (32) but with ω_o' instead of ω_o . Hence, in general,

$$I(\omega) = \frac{1}{3\pi^2 c^2} \omega^2 \underbrace{W}_{\text{Average energy of the oscillator at temperature } T} \quad (32)'$$

Required *light intensity spectral density* $I(\omega)$ inside the box at temperature T in order to maintain equilibrium.

Notice

$$\text{Units of } [I(\omega) d\omega] = [\text{Intensity}] = \frac{J}{m^2 s}$$

$$\text{Units of } [I(\omega)] = \frac{[\text{Intensity}]}{[\Delta\omega]} = \frac{J/(m^2 s)}{1/s} = \frac{J}{m^2}$$

It is worth to highlight that,

- Expression (32)' has remained undisputed. That is, it is still considered correct even when the new quantum mechanics concepts are introduced.
- It is in the calculation of the average energy \bar{W} where the classical and quantum approaches fundamentally diverge.

3.1.C.b Classical calculation of the atom's average energy \bar{W} .

In classical statistical mechanics there exists a very general result so called “equipartition theorem,” which states that the mean value of a quadratic term in the energy is equal to $\frac{1}{2} k_B T$. Here k_B is the Boltzmann's constant and T is the absolute temperature.

The Boltzmann distribution

The equipartition theorem can be obtained from the Boltzmann's probability distribution for a small system \mathcal{A} in equilibrium with a (huge) reservoir at temperature T . The Boltzmann distribution states that the probability that the system S be found in a state of energy E is proportional to $e^{-E/k_B T}$; that is ,

$$\begin{aligned} P(E) &\propto e^{-E/k_B T} \\ &= C e^{-E/k_B T} \quad \text{probability to find the system} \quad (33) \\ &\quad \text{A in a state of energy } E \end{aligned}$$

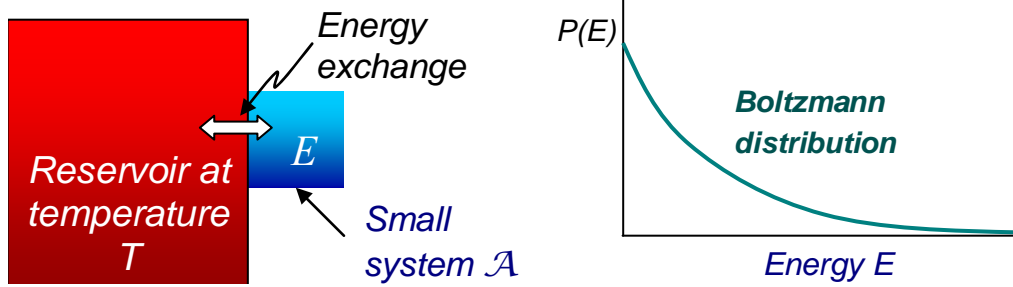


Fig 3.13 Left: A system interacting with a thermal reservoir. **Right:** Boltzmann's distribution to find the system in a state of energy E .

The values of E could go from 0 to infinity (the reservoir being in charge of keeping the temperature constant); but, as the expression above indicates, the states of lower energy have a higher probability. Since for a given energy there may be several states characterized by the same energy, it is usual to define,

$$g(E)dE \quad \text{number of states with energy } E, \text{ within an interval } dE, \quad (34)$$

thus giving

$$Ce^{-E/k_B T} g(E)dE \quad \text{probability to find the system } \mathcal{A} \text{ in a state of energy between } E \text{ and } E + dE,$$

which suggests to rather identify a probability-density $\mathcal{P}(E)$ defined as follows

$$\mathcal{P}(E)dE = Ce^{-E/k_B T} g(E)dE \quad \text{the probability to find the system in a state of energy between } E \text{ and } E + dE, \quad (35)$$

with C being a constant to be determined.

Since the probabilities added over all the possible states should be equal to 1, we must require, $\int_0^\infty Ce^{-E'/k_B T} g(E')dE' = 1$, which gives,

$$C^{-1} = \int_0^\infty e^{-E'/k_B T} g(E')dE' \quad (36)$$

A self consistent expression for $P(E)$ is therefore given by,

$$\mathcal{P}(E)dE = \frac{e^{-E/k_B T} g(E)dE}{\int_0^\infty e^{-E'/k_B T} g(E')dE'} \quad (37)$$

(Notice in the denominator we are using a 'dummy' variable E' .)

From expression (37) we can formally calculate the average energy of the system,

$$\langle E \rangle = \frac{\int_0^\infty E e^{-E/k_B T} g(E)dE}{\int_0^\infty e^{-E'/k_B T} g(E')dE'} \quad (38)$$

The Equipartition Theorem

It turns out, very often the energy of the system may contain a quadratic term. Consider for example

$$E = \frac{p_x^2}{2m} + \frac{1}{2} kx^2 + \dots ,$$

and we would like to calculate, for example, the average value of the

kinetic energy term $\frac{p_x^2}{2m}$ alone. As we know, being the system in

contact with a heat reservoir, the value of $\frac{p_x^2}{2m}$ is sometimes high, sometimes it is low because it gains or loses energy from the heat reservoir; we would like to know what would be its average value

$$\left\langle \frac{p_x^2}{2m} \right\rangle .$$

$$\left\langle \frac{p_x^2}{2m} \right\rangle = \frac{\int_0^\infty \frac{p_x^2}{2m} e^{-\frac{p_x^2}{2m}/k_B T} dp_x}{\int_0^\infty e^{-\frac{p_x^2}{2m}/k_B T} dp_x} \quad (39)$$

Let's call

$$\beta = \frac{1}{k_B T} \quad (40)$$

In terms of β expression (39) becomes,

$$\begin{aligned} \left\langle \frac{p_x^2}{2m} \right\rangle &= \frac{\int_0^\infty \frac{p_x^2}{2m} e^{-\beta \frac{p_x^2}{2m}} dp_x}{\int_0^\infty e^{-\beta \frac{p_x^2}{2m}} dp_x} = \frac{\int_0^\infty -\frac{\partial}{\partial \beta} e^{-\beta \frac{p_x^2}{2m}} dp_x}{\int_0^\infty e^{-\beta \frac{p_x^2}{2m}} dp_x} = \frac{-\frac{\partial}{\partial \beta} \int_0^\infty e^{-\beta \frac{p_x^2}{2m}} dp_x}{\int_0^\infty e^{-\beta \frac{p_x^2}{2m}} dp_x} \\ \left\langle \frac{p_x^2}{2m} \right\rangle &= -\frac{\partial}{\partial \beta} \ln \left[\int_0^\infty e^{-\beta \frac{p_x^2}{2m}} dp_x \right] \end{aligned} \quad (41)$$

Defining the variable $u \equiv \sqrt{\frac{\beta}{2m}} p_x$,

$$\left\langle \frac{p_x^2}{2m} \right\rangle = -\frac{\partial}{\partial \beta} \ln \left[\sqrt{\frac{2m}{\beta}} \int_0^\infty e^{-u^2} du \right] = -\frac{\partial}{\partial \beta} \ln \left[\sqrt{\frac{1}{\beta}} \sqrt{2m} \int_0^\infty e^{-u^2} du \right]$$

$$\left\langle \frac{p_x^2}{2m} \right\rangle = -\frac{\partial}{\partial \beta} \left[\ln \left(\sqrt{\frac{1}{\beta}} \right) + \underbrace{\ln \left(\sqrt{2m} \int_0^\infty e^{-u^2} du \right)}_{\text{Term independent of } \beta} \right]$$

$$\left\langle \frac{p_x^2}{2m} \right\rangle = -\frac{\partial}{\partial \beta} \left[-\frac{1}{2} \ln \beta \right] = \frac{1}{2\beta}$$

$$\left\langle \frac{p_x^2}{2m} \right\rangle = \frac{1}{2} k_B T \quad (42)$$

Had we chosen any other quadratic term of the energy we would have obtained the same result. This is the equipartition theorem. It states that the mean value of each independent quadratic term in the energy is equal to $\frac{1}{2} k_B T$.

The ultraviolet catastrophe

Using this result (42) in expression (32) $I(\omega_o) = \frac{1}{3\pi^2 c^2} \omega_o^2 W$, the different degrees of freedom (let's assume there are f different quadratic terms in the expression for the total energy) involved in the

calculation of W would lead to a finite number f of $\frac{1}{2}k_B T$. Thus,

$I(\omega_o) = \frac{1}{3\pi^2 c^2} \omega_o^2 f \frac{1}{2} k_B T$. Since the value of ω_o is accidental (we would obtain a similar expression if we were to choose an atom of different resonance frequency), we have the following result,

$$I(\omega) = \frac{f k_B T}{6\pi^2 c^2} \omega^2 \quad \text{classical prediction} \quad (43)$$

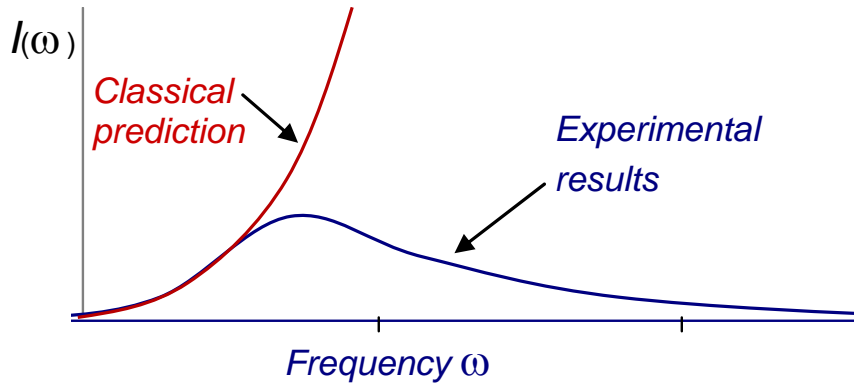


Fig. 3.14 The serious discrepancy between the experimental results and the theoretical prediction is called *the ultraviolet catastrophe*.

3.1.D The birthday of Quantum Physics: Planck's Hypothesis to calculate the atom's average energy W

To bring the theoretical prediction closer to the experimental results Planck considered the possibility of a violation of the law of equipartition of energy described above. Rather than using expression (43), the starting expression would be expression (32)

$I(\omega) = \frac{1}{3\pi^2 c^2} \omega^2 W$, with the average energy of the oscillator W no to have a constant value (as the equipartition theorem predicted) but rather being a function of the frequency, $W(\omega)$, with the following requirements,

$$\omega^2 W(\omega) \xrightarrow{\omega \rightarrow 0} 0$$

and

$$\omega^2 W(\omega) \xrightarrow{\omega \rightarrow \infty} 0$$

(44)

For the statistical calculation of W ,

Planck did not question the classical Boltzmann's Statistics described in the section above; that would still be considered valid. (45)

Planck realized that he could obtain the desired behavior expressed in (44) if,

- rather than treating the energy of the oscillator as a continuous variable, the energy states of the oscillator should take only discrete values:

$$0, \varepsilon, 2\varepsilon, 3\varepsilon, \dots \quad (46)$$

- the energy steps would be different for each frequency

$$\varepsilon = \varepsilon(\omega) \quad (47)$$

where the specific dependence of ε in terms of ω to be determined

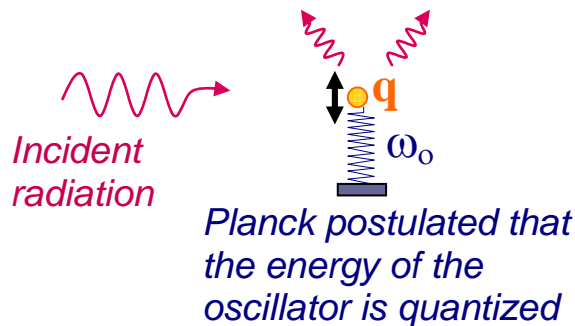


Fig. 3.15 An atom receiving radiation of frequency ω , can be excited only by discrete values of energy $0, \varepsilon, 2\varepsilon, 3\varepsilon, \dots$

According to Planck, in the classical integral expression (37)

$$W_{\text{classical}} = \langle E \rangle = \frac{\int_0^\infty E e^{-E/k_B T} g(E) dE}{\int_0^\infty e^{-E'/k_B T} g(E') dE'}, \text{ one would have to replace:}$$

$g(E)dE = 1$ [$g(E)dE$ gives the number of states with energy E within an interval dE]

$$dE \rightarrow \varepsilon$$

$$\int_0^{\infty} dE \rightarrow \sum_{n=0}^{\infty}$$

thus obtaining,

$$W_{Planck}(\omega) = \langle E \rangle = \frac{\sum_{n=0}^{\infty} E_n e^{-E_n / k_B T}}{\sum_{n=0}^{\infty} e^{-E_n / k_B T}} \quad (48)$$

where $E_n = n \varepsilon(\omega)$; $n = 1, 2, 3, \dots$

A graphic illustration can help understand why this hypothesis could indeed work:

- First we show how classical physics evaluate the average energy.

$$\langle E \rangle_{classical} = \int_0^{\infty} E [P(E)] dE = \text{area under the curve } EP(E)$$

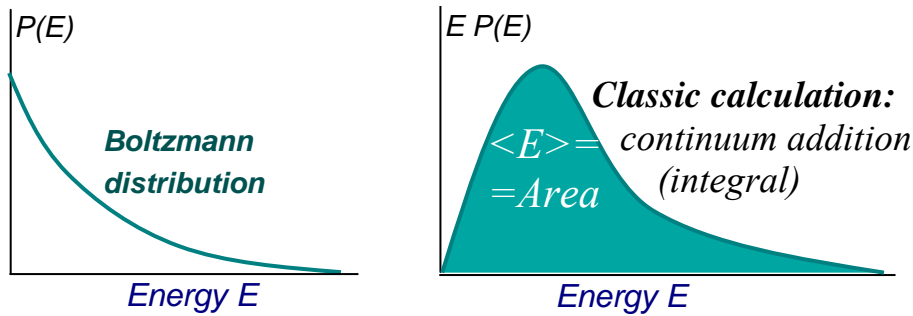


Fig. 3.16 Schematic representations to calculate the average energy of the oscillator under a classical physics approach.

- Using **Plank's hypothesis** $\langle E \rangle_{Planck} = \sum_{n=0}^{\infty} E_n P(E_n)$

➤ **Case: Low frequency values of ω**

For this case, Planck assumed ε should have a small value (for the reasons explained in Fig. 3.17).

$$\varepsilon \approx \text{small value} \quad (49)$$

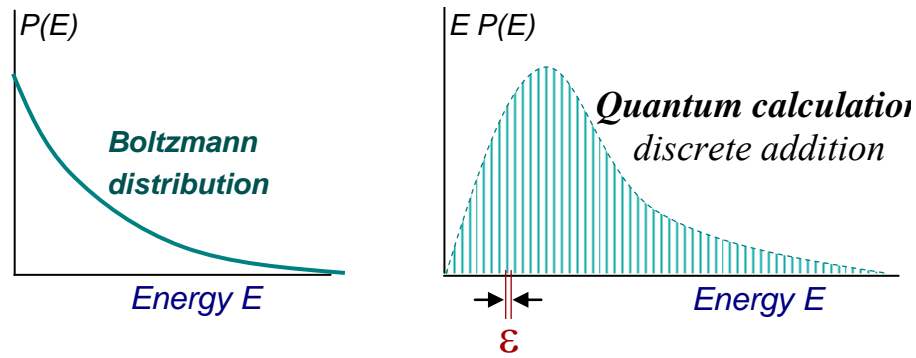


Fig. 3.17 Schematic representations to calculate the average energy of the oscillator assuming the oscillator can admit only discrete values of energy, for the case where the separation ε between contiguous energy levels being of relatively low value.

Indeed, comparing Fig. 3.16 and Fig 3.17 one notices that if ε is small then the value of $\sum_{n=0}^{\infty} E_n P(E_n)$ will be very close to the classical value.

It is indeed desirable that Planck's results agree with the classic results at low frequencies, since the classical predictions and the experimental results agree well at low frequencies (see Fig. 3.14 above.)

➤ **Case: High frequency values of ω**

For this case, Planck assumed, Planck assumed ε should have a bigger value

$$\varepsilon \approx \text{big value} \quad (50)$$

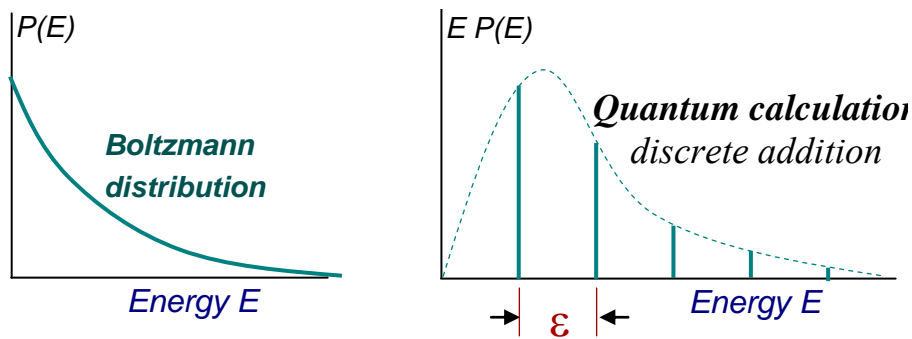


Fig. 3.18 Schematic representations to calculate the average energy of the oscillator assuming the oscillator can admit only discrete values of energy, for the case where the separation ε between contiguous energy levels being of relatively large value.

Notice in this case, the value of $\langle E \rangle_{Planck} = \sum_{n=0}^{\infty} E_n P(E_n)$ (depicted in Fig. 3.17) will be very different from the one depicted in Fig. 3.18 (the latter closer to the classical result .)

In fact, $\sum_{n=0}^{\infty} E_n P(E_n)$ tends to zero as the step ε is chosen larger.

This result is desirable, since the experimental result indicate that $\langle E \rangle$ tends to zero at high frequencies.

It appears then that the Planck's model (48) could work. Now, which function $\varepsilon(\omega)$ could be chosen such that

$\varepsilon(\omega)$ is small at low ω , and large at large ω ?

An obvious simple choice is to assume a linear relationship,

$$\varepsilon(\omega) = \hbar \omega \quad (51)$$

where \hbar is a constant of proportionality to be determined.

Replacing (51) in (48) one obtains,

$$W_{Planck}(\omega) = \langle E \rangle = \frac{\sum_{n=0}^{\infty} E_n e^{-E_n / k_B T}}{\sum_{n=0}^{\infty} e^{-E_n / k_B T}} = \frac{\sum_{n=0}^{\infty} n \hbar \omega e^{-n \hbar \omega / k_B T}}{\sum_{n=0}^{\infty} e^{-n \hbar \omega / k_B T}}$$

Let $\alpha \equiv \frac{\hbar}{kT}$

$$W_{Planckl}(\omega) = \frac{kT \sum_{n=0}^{\infty} n \alpha \omega e^{-n \alpha \omega}}{\sum_{n=0}^{\infty} e^{-n \alpha \omega}} = \frac{-kT \sum_{n=0}^{\infty} \alpha \frac{\partial}{\partial \alpha} e^{-n \alpha \omega}}{\sum_{n=0}^{\infty} e^{-n \alpha \omega}}$$

Since $d[\ln(u)]/dx = (1/u) du/dx$

$$W_{Planckl}(\omega) = -kT \alpha \frac{\partial}{\partial \alpha} \ln \left[\sum_{n=0}^{\infty} e^{-n \alpha \omega} \right]$$

If we define $x = e^{-\alpha \omega}$, then

$$\sum_{n=0}^{\infty} e^{-n \alpha \omega} = 1 + x + x^2 + x^3 \dots$$

This series is equal to $1/(1-x)$

$$= \frac{1}{1-x} = \frac{1}{1-e^{-\alpha \omega}}$$

$$W_{Planckl}(\omega) = -kT \alpha \frac{\partial}{\partial \alpha} \ln \left[\sum_{n=0}^{\infty} e^{-n \alpha \omega} \right] = -kT \alpha \frac{\partial}{\partial \alpha} \ln \left[\frac{1}{1-e^{-\alpha \omega}} \right]$$

$$= kT \alpha \frac{\partial}{\partial \alpha} \ln [1 - e^{-\alpha \omega}]$$

$$= kT \alpha \frac{\omega e^{-\alpha \omega}}{1 - e^{-\alpha \omega}} = kT \alpha \omega \frac{1}{e^{\alpha \omega} - 1}$$

$$W_{Planckl}(\omega) = \hbar \omega \frac{1}{e^{\hbar \omega / kT} - 1} \quad (52)$$

Notice: $W_{Planckl}(\omega) \xrightarrow{\omega \rightarrow 0} kT$

$$W_{Planckl}(\omega) \xrightarrow{\omega \rightarrow \infty} 0$$

With this result, expression (33) becomes

$$I(\omega) = \frac{1}{3\pi^2 c^2} \omega^2 W_{Planck} \quad (53)$$

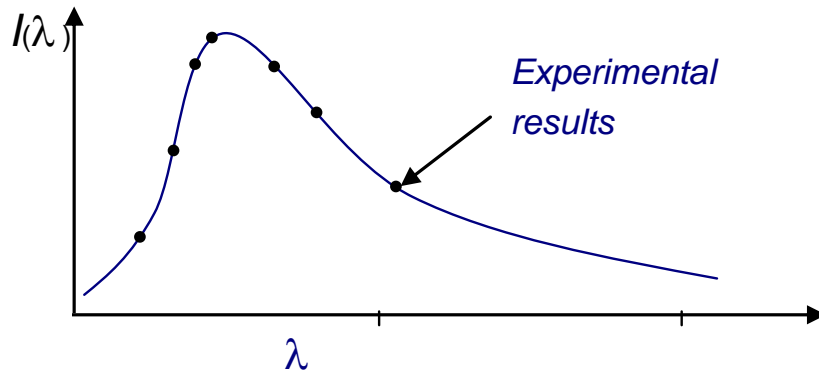


Fig. 3.19 Planck's model quantization of the oscillator energy fits well the experimental results.

Particle's and wave's energy quantization

- Historically. Planck initially (1900) postulated only that the energy of the oscillating particle (electrons in the walls of the blackbody) is quantized. The electromagnetic energy, once radiated, would spread as a continuous.
- It was not until later that Plank accepted that the oscillating electromagnetic waves were themselves quantized. The latter hypothesis was introduced by Einstein (1905) in the context of explaining the photoelectric effect, which was corroborated later by Millikan (1914).

3.1.B.g Light Energy Density $U(\omega)$ at equilibrium.

The Concept of Electromagnetic Modes

(see "Complement Chapter-3" notes (website))

3.2 PARTICLE-LIKE PROPERTIES of RADIATION

3.2.A Processes involving the absorption or scattering of radiation by particles

3.2.A.a Photoelectric effect Einstein's hypothesis of the quantized radiation energy

Einstein's interpretation:

- In the *wave* picture, the intensity of radiation is given by the average of the Poynting vector **S**,

$$I = \langle S \rangle = \langle \epsilon_0 c E^2 \rangle$$

where E is the electric field of the wave

In the *particle* picture, the intensity is written as

$$I = N h \gamma$$

where N is the number of photons per unit time crossing a unit area perpendicular to the direction of propagation

Einstein suggested that $\langle E^2 \rangle$ could be interpreted as a measure of the average number of photons per unit volume.

- The radiation granularity concept leads to consider the light intensity as a statistical variable

A light source emits photons randomly in all directions

The exact number of photons crossing an area fluctuates (around an average number) in time and space

3.2.A.b The Compton Effect

Scattering of a complete quantum of radiation in definite direction.

Compton explained the results on the assumptions that

- each electron scatters a complete quantum of radiation (photon); and
- the quanta of radiation are received from definite directions and are scattered in definite directions

3.3 WAVE-LIKE PROPERTIES of PARTICLES

3.3.A The Louis de Broglie Hypothesis

- The Compton's Effect experiment had provided strong evidence on the **particle nature of radiation**. The typical **symmetry** expressed by *Nature* in many physical processes (for example, charges in motion produce magnetism and magnets in motion produce currents) may have led Louis de Broglie to propose the **wave nature of particles**.

- In 1924, Louis de Broglie, using arguments based on the properties of **wave packets**, proposed that,

$$\left. \begin{array}{l} \text{the wave aspect of matter are related to its particle} \\ \text{aspect in exactly the same quantitative way displayed by} \\ \text{radiation.} \\ \lambda = h / p \quad \text{where } \lambda \text{ is the wavelength of the wave} \\ \quad \quad \quad \text{associated with the particle's motion; and} \\ \gamma = E / h \quad \text{the total energy } E \text{ is related to the frequency} \\ \quad \quad \quad \gamma \text{ of the wave associated with its motion.} \end{array} \right\} (66)$$

Here h is the Planck's constant; $h = 6.6 \times 10^{-34} \text{ Js}$.

Since in the case of radiation ($mass \ m = 0$) we already know that $\lambda \gamma = c$, only one of the relationships above is needed to obtain both λ and γ from its energy and momentum's particle properties.

In contrast, for a particle of mass $m \neq 0$, one needs both relationships given above to obtain the corresponding λ and γ .

- Order of magnitude calculation of $\lambda_{de \ Broglie}$

Case: $m = 10^{-3} \text{ Kg}$, $v = 1 \text{ m/s}$

$$p = mv = 10^{-3} \text{ Kg} \cdot \text{m/s}$$

$\lambda = h/p = 6.6 \times 10^{-31} \text{ m}$. This value is inaccessible to any measurement currently possible

Case: $m_e = \text{electron's mass} = 9.1 \times 10^{-31} \text{ Kg}$, $q_e = 1.6 \times 10^{-19} \text{ C}$

If the electron accelerated through a potential difference of V_o volts its kinetic energy will be determined by

$$q_e V_o = p^2 / 2m, \text{ which gives } p = (2m_e q_e V_o)^{1/2}$$

$$\text{For } V_o = 50 \text{ Volts: } p = (2m_e q_e V_o)^{1/2} = (14.56 \times 10^{-48})^{1/2}$$

$$p = 3.8 \times 10^{-24} \text{ m/s}$$

$$\lambda = h / p = (6.6 \times 10^{-34} \text{ J} \cdot \text{s}) / (3.8 \times 10^{-24} \text{ m/s}) = 1.7 \times 10^{-10} \text{ m}.$$

This value is of the same order of magnitude of the X-rays' wavelength.

3.3.B Experimental confirmation of the de Broglie hypothesis. Electron Diffraction

- In 1897 J. J. Thompson discovered the electron (establishing the ratio q_e / m_{e^-}) and was awarded the Nobel Prize in 1906.
- The de Broglie wavelength $\lambda_{de\ Broglie}$ associated to an electron falls in the order of Angstroms (when accelerated at moderate voltages ~ 50 Volts, as shown in the example above), which happens to be the inter-atomic spacing in a crystalline solid.
- In 1926 Elsasler suggested that the wave nature of particles could be tested by verifying whether or not electrons of the proper energy are diffracted by a crystalline solid. This idea was confirmed by Davisson and Germer (in the United States) and J. J. Thompson's son G. P. Thompson in Scotland (1927).

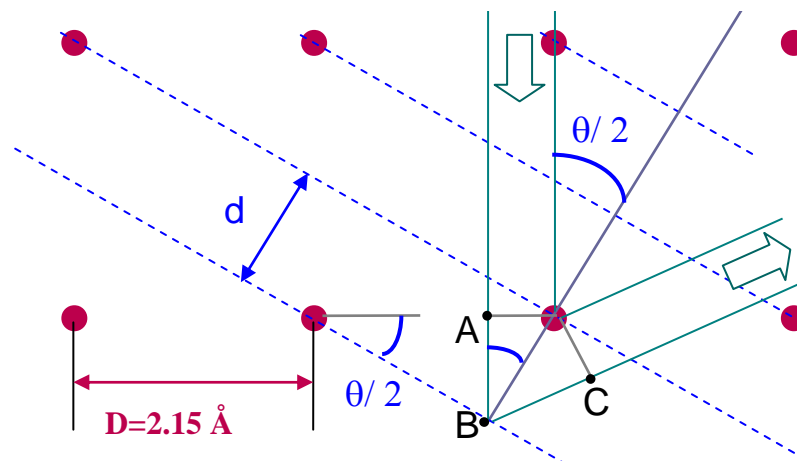
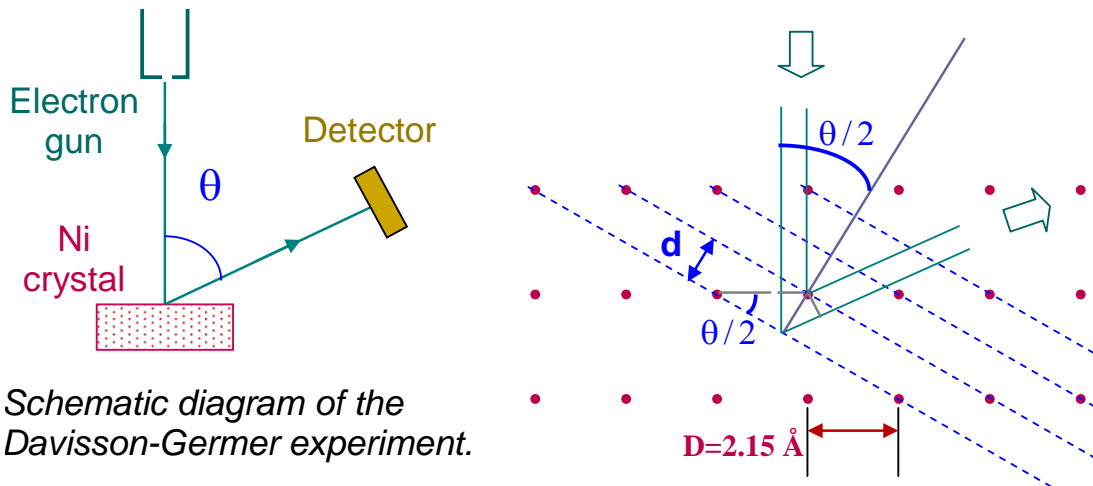


Fig. 3.19 Experimental setup for demonstrating the wave character of electrons

If the incident electrons were interpreted as waves of wavelength λ , reflecting from the Bragg's planes (similar to the x-rays), then they could give rise to interference phenomena. In particular, the condition for obtaining constructive interference (see figure above) is given by *length of path* $ABC = n\lambda$; or,

$$2d \cos(\theta/2) = n\lambda \quad (n=1,2, \dots)$$

From the figure above, $d = D \sin(\theta/2)$. Thus the condition of constructive interference becomes $2D \sin(\theta/2) \cos(\theta/2) = n\lambda$, or

$$D \sin(\theta) = n\lambda \quad (n=1,2, \dots) \quad (67)$$

For an accelerating voltage $V_0 = 54$ volts, $\lambda_{\text{de Broglie}} = h/p = 1.66 \text{ \AA}$ (as calculated above). According to expression (46) it would be expected to observe a maximum of interference at,

$$\sin(\theta) = \lambda/D = 1.66/2.15 = 0.77$$

$$\theta = 50.3 \text{ degrees} \quad (\text{theoretical prediction.})$$

The figure below shows a schematic of the experimental result obtained by Davisson and Germer.

The peak signal of detected electrons around $\theta = 50^\circ$ supports the de Broglie hypothesis, since it can be explained as *constructive interference of waves scattered by the periodic arrangement of the atoms in the crystal*

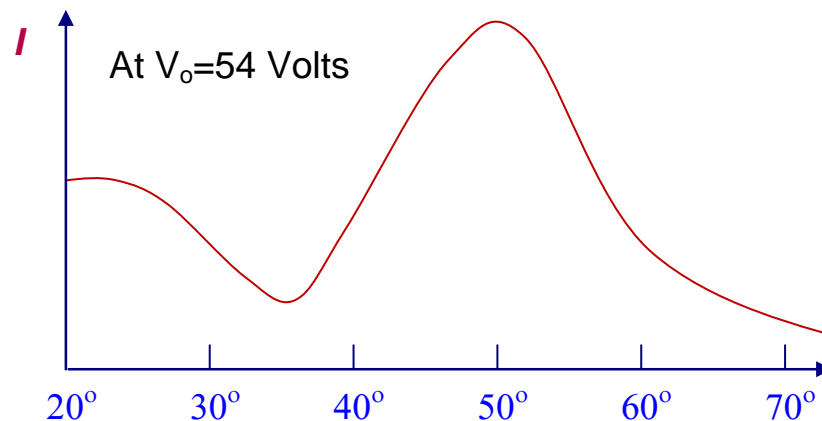


Fig. 3.20 Experimental results obtained by Davisson and Germer. Collector current I as a function of the detector's angle (for a fixed value of the accelerating voltage)

- The electron interference is not between waves associated with one electron, and waves associated with another. Instead, it is the interference between different parts of the wave associated with a single electron.

The above can be demonstrated by using an electron gun of such low intensity that **one electron at a time incident the crystal** and by showing that the pattern of scattered electrons remains the same.

3.4 WAVE-PARTICLE DUALITY

- Not only electrons but all materials, charge or uncharged, show wavelike characteristics:

Estermann, Stern, and Frish

Molecular beams of hydrogen and atomic beams of helium from a lithium fluoride crystal. The difficulties of these experiments lie in the low intensity of the molecular beams attainable.

Fermi. Marshall and Zinn

Use the abundant slow neutrons available from nuclear reactors. (X-ray analysis is based on the photon-electron interaction; neutrons rather interact with the nucleus.)

- The particle aspect is emphasized when studying their emission and detection

The wave aspect is emphasized when studying their motion

- The small value of h impedes the observation of wave-particle duality in the macroscopic world.

Since $\lambda = h / p$, a zero value for h would imply an absence of diffraction effects. On the other hand, the (relatively) large

momentum of macroscopic objects compared to h also makes λ too small to be detected.

- The deeper understanding of the link between the wave model and the particle model is provided by a probabilistic interpretation of the wave-particle duality:
 - In the case of **radiation**, it was Einstein who united the wave and particle theories (used in the explanation of the photoelectric effect.)
 - Max Born (many years after) applied later similar arguments to unite the wave and particle theories of **matter**. (Einstein, however, did not accept it.)

This latter aspect is more involved and becomes the subject of the next chapter.

Overlook the following APPENDIX

- **The electromagnetic damping constant**

➤ For comparison, let's consider first the case of a dissipative force proportional to the velocity $F_{dis} \equiv -m \gamma \frac{dx}{dt}$,

The Eq. of motion is $m \frac{d^2x}{dt^2} + kx = F_{ext}$, which can be expressed in terms of energy balance as follows ,

$$\frac{d}{dt} \left[\frac{1}{2} m \left(\frac{dx}{dt} \right)^2 + \frac{1}{2} kx^2 \right] = P_{ext}(t) - m\gamma \left(\frac{dx}{dt} \right)^2 \quad (41)$$

For $x = x_o e^{j\omega t}$, the average dissipating power is given by,

$$\begin{aligned} \langle P_{dis} \rangle &= \langle F_{dis} \frac{dx}{dt} \rangle = \langle (-m\gamma \frac{dx}{dt}) \frac{dx}{dt} \rangle = -m\gamma \langle \left(\frac{dx}{dt} \right) \left(\frac{dx}{dt} \right)^* \rangle \\ &= -m\gamma \left[\frac{1}{2} \frac{dx}{dt} \left(\frac{dx}{dt} \right)^* \right] = -\frac{1}{2} m\gamma \omega^2 x_o (x_o)^* \\ \langle P_{dis} \rangle &= -\frac{1}{2} m\gamma \omega^2 |x_o|^2 \end{aligned} \quad (42)$$

The average total mechanical energy of the oscillator varies as,

$$\left\langle \frac{d}{dt} \left[\frac{1}{2} m \left(\frac{dx}{dt} \right)^2 + \frac{1}{2} kx^2 \right] \right\rangle = \langle P_{ext}(t) \rangle - \frac{1}{2} m\gamma \omega^2 |x_o|^2 \quad (43)$$

➤ For a charge q oscillating according to $x = x_o e^{j\omega t}$, the average electromagnetic energy dissipated is given by,

$$\left\langle \frac{d}{dt} \left[\frac{1}{2} m \left(\frac{dx}{dt} \right)^2 + \frac{1}{2} kx^2 \right] \right\rangle = \langle P_{ext}(t) \rangle - \frac{q^2 \omega^4}{12\pi\epsilon_o c^3} |x_o|^2$$

For the sake of comparison of the effective dissipation energy between the mechanical dissipation and electromagnetic dissipation cases, the following definition is typically introduced,

$$\begin{aligned} \frac{1}{2} m \gamma_{electromagnetic} \omega^2 &\equiv \frac{q^2 \omega^4}{12\pi\epsilon_o c^3} \\ \gamma_{electromagnetic} &\equiv \frac{q^2 \omega^2}{6m\pi\epsilon_o c^3} = \frac{2}{3c} \frac{q^2 / (4\pi\epsilon_o)}{mc^2} \omega^2 \end{aligned} \quad (44)$$

Thus

$$\left\langle \frac{d}{dt} \left[\frac{1}{2} m \left(\frac{dx}{dt} \right)^2 + \frac{1}{2} kx^2 \right] \right\rangle = \langle P_{ext}(t) \rangle - \frac{1}{2} m \gamma_{electromagnetic} \omega^2 |x_o|^2 \quad (45)$$

Note: When a external source is present and makes the charge oscillate at $\omega \neq \omega_o$ we have to use

$$\left\langle \underbrace{\frac{d}{dt} \left[\frac{1}{2} m \left(\frac{dx}{dt} \right)^2 + \frac{1}{2} k x^2 \right]}_W \right\rangle = \langle P_{ext}(t) \rangle - \frac{1}{2} m \gamma_{electromagnetic} \omega^2 |x_o|^2$$

which is essentially,

$$\frac{\Delta W}{\Delta t} = \langle P_{ext}(t) \rangle - \frac{1}{2} m \gamma_{electromagnetic} \omega^2 |x_o|^2$$

Notice this term $\frac{1}{2} m \omega^2 |x_o|^2$ is smaller than W , and since $|x_o|^2$ is also much smaller than the amplitude at resonance, therefore the loss of energy outside the resonance frequency is **comparatively very small**.

¹ R. Eisberg and R. Resnick, "Quantum Physics," 2nd Edition, Wiley, 1985. See Chapter 1

² Feynman Lectures, Vol - I, Chapter 32