The reasons of Quantum Mechanics

In 1888 a Swedish researcher called Rydberg was observing the emission lines of several materials. He noticed that colored lines are emitted with some regularity, and he though there should be a way to predict the position of each line at wavelength λ with a single formula. After several trials using hidrogen gas, he finally found this formula:

$$\frac{1}{\lambda} = R(\frac{1}{n_f} - \frac{1}{n_i}) \tag{1}$$

This is called it Rydberg formula and predict the exact position of hydrogen emission lines, the very important fact is that there are these strange numbers n_i and n_f, that now we call *radial quantum number* that were consecutive integer number of a then called *series* of lines.

This fact discovered in 1888, was again put forward later by the experiments of the British Rutherford. Rutherford in 1911 irradiated with alpha particles (two protons and two neutrons) a gold foil. With his surprise he found that almost all particles went straight through the gold, like he was inconsistent, but in some rare case, the particle was rejected back, like she collided with something very heavy. He made several calculations that pointed that the atom of gold were almost completely empty, and all the mass was concentrated in a heavy positive charged *atomic nucleus.* Then he developed his own simple model of atom, a sort of planetary system, were negatively charged electrons have almost no mass and they were orbiting a central heavy nucleus.

Later Bohr and Rutherford developed the so called *Rutherford-Bohr model of the atom.* This model is very similar to the planetary model firstly introduced by Rutherford, but electrons were kept at fixed orbits in such a way that the Rydberg formula can be satisfied.

Why electrostatic forces kept negative electrons in this fixed orbits, without radiating energy and without being attracted end collapsing to the positive nucleus was still a mystery.

Another phenomena was suggesting the presence of a *new physics.* If we illuminate a metal, like Zinc for example, it was possible to observe the emission of electron. This was firstly observed by Hertz, and was actually called Hertz effect. The strange thing was that there was a sort of *threshold* of wavelength under which no emission was possible. If the wavelength of the radiation was bigger than this value, there was no electron emission from the metal *even increasing the light intensity.* This phenomena was impossible to explain with classical physics, because the energy of an oscillator (Maxwell showed in 1861 that the electromagnetic field is mathematically equivalent to an oscillator) should be proportional to its amplitude. If I increase the amplitude, I should get electron out sooner o later (!) However, no electron was emitted, whatever intensity, if frequency (the inverse of the wavelength) was over the threshold. Moreover, even if light had the same intensity, changing increasing the frequency was increasing the electron emission ! What was happening here ?

Einstein explained that the energy of light is divided in tiny *quanta* of energy, and introduced for the first time the basic quantum mechanics concepts in the effort to explain the photoelectric effect. However, his theory was not widely accepted and remained controversial for many years.

The Black Body radiation, the first Quantum Mechanics Formula

Suppose we want to study the radiation emission of a hot body. In a hot body, all the molecules vibrates. We can approximate these vibrations as elastic oscillations of a mass particle. If there is radiation emission, it means this particle is charged. It is known to physicists that a charged particle oscillating radiate away an amount of energy proportional to the energy of the particle, accordingly to this formula:

$$I = \frac{dW}{dt} \propto \gamma W \tag{2}$$

This means that the energy radiated away per unit of time is proportional to the energy of the charge with a coefficient γ. On average, at a certain temperature T the energy of the particle is known to be $K_B T$, so we have:

$$\frac{dW}{dt} \propto \gamma K_B T \tag{3}$$

We do not derive here the detail of the calculations, however γ is ω/Q where Q is the oscillation *quality factor.* This quality factor is proportional to $1/\omega$. If so

$$\gamma \propto \omega^2$$

Finally we find in the relation for the intensity $I(\omega)$ a direct dependence with ω^2 and the molecules kinetic energy: kT,

$$I(\omega) \propto \omega^2 K_B T \tag{4}$$

this equation is called the *Rayleigh's law* for the *black body* radiation. Interestingly enough, this equation fits very well the experimental data for low energies, however, it fail completely to predict a diminished emission at higher energies. Accordingly to eq. 4, because of the ω^2, we should observe a lot of X-Ray and other unhealthy emission from a hot body, much more UV and X-rays than other radiation! Instead, of course, in the experiments, we never observe emission over UV or X-rays, even if we heat-up a body at very high temperatures. Moreover, a low without w^2 will be in conflict with the conservation of energy, that would be very bad indeed! There must be something wrong in this equation, what is going on here ?!? Many researchers at that time studied the problem, and nobody was able to find an answer. The problem was called by physicists of the time *the UV catastrophe*. Max Planck also studied the problem and was getting mad at it. Inspired by Rutherford-Bohr model of the atom, where electrons stay in a fixed orbit regulated by *quantum* numbers, one day he made the very fancy hypothesis that the kinetic energy cannot be a continuous value, but must be quantized in multiple steps of $h\omega$. In this way he calculated the average energy that is not any more kT as in the equation 4, but a different value that drops down very fast at higher frequencies. This supposition that Energy cannot be continuous, was defined by Planck and his colleagues as an *act of desperations* ! How it was done ?

Planck thought that for some reason, the oscillation of electrons must be *quantized*, exactly as the strings of a guitar are forced to vibrate only to multiple frequencies. This idea was not unfamiliar to physicists, in fact standing waves in musical instruments behave exactly this way: frequency is *quantized* in multiples of a base tone (see fig. 1)

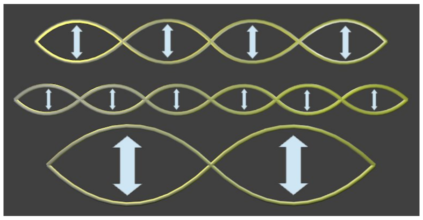

Fig. 1. Examples of *standing waves* of a string at different frequencies. The arrows represent the position of the string at the minimum and maximum of the oscillation.

Planck thought then that the vibration of the molecules in a hot body, must behave exactly this way. So he simply calculated the average energy of such systems. The average energy is : $<E>=\frac{E_{tot}}{N_{tot}}$ where E_{tot} is the total energy of the system, and N_{tot} is the total number of available *states*.

Let's calculate first N_{tot}: lets choose one frequency ω. For this single ω, if we have many possible levels of energies E_0, E_1, E_2 etcetera. Each of this has energy multiple of the minimum E_0, in this succession: $E_1 = h\omega$, $E_2 = 2h\omega$, $E_3 = 3h\omega$ etcetera.

We will have N_0, N_1, N_2 molecules on each of these energy levels, right? The problem now is: "what will be the *distribution* of these energies?", in other words, how many molecules will be in N_0, N_1, N_2 and so on? Of course, Planck wanted to be simple and he thought at the well known Boltzmann distribution that we know very well. So he said, the number of molecules in each energy states E_0, E_1, $E_2 \ldots$, will be distributed as a Boltzmann distribution, so like this :

$$\begin{aligned} &N_0 \\ N_1 = N_0 e^{-E_1/kT} &= N_0 e^{-h\omega/kT} \\ N_2 = N_0 e^{-E_2/kT} &= N_0 e^{-2h\omega/kT} \\ N_3 = N_0 e^{-E_3/kT} &= N_0 e^{-3h\omega/kT} \\ &\ldots \end{aligned} \tag{5}$$

where h is a constant. If we have an infinite number of these states, what is the total N_{tot} that we are looking for ? Well, let's simplify the equation by calling $x = e^{-h\omega/kT}$, then our eq. 6 becomes:

$$\begin{aligned} &N_0 \\ N_1 &= N_0 x \\ N_2 &= N_0 x^2 \\ N_3 &= N_0 x^3 \\ &\ldots \end{aligned} \tag{6}$$

and so on. Then the total N_{tot} is

$$N_{tot} = N_0(1 + x + x^2 + x^3 + \ldots)$$

For the theory of series it is very easy to demonstrate (simply multiply the series by x and compare it with itself) that

$$N_{tot} = N_0 \frac{1}{1-x} \tag{7}$$

At this point we only need to calculate the total energy of the system. Planck simply added up the energy for each level. The total Energy at the lowest *ground* level was for simplicity set to zero, the total energy at the fist level was $N_1 * E_1$, for the second $N_2 * E_2$ and so on... since Planck assumed that energy proceed in multiple of a base (*ground*) value $E_0 = h\omega$, then $E_1 = 2h\omega$, $E_3 = 3h\omega$. If we proceed this way, using again $x = e^{-h\omega/kT}$ the total energy is then

$$E_{tot} = h\omega(x + 2x^2 + 3x^3 + \ldots) \tag{8}$$

Again, if this series is infinite, the theory says that (use the fact that $x + x^2 + x^3 + \ldots \approx x/(1-x)$)

$$E_{tot} = h\omega \frac{x}{(1-x)^2} \tag{9}$$

so the average system energy that we are looking for is:

$$< E_k >= \frac{E_{tot}}{N_{tot}} = h\omega \frac{x}{1-x} \tag{10}$$

or substituting back x

$$< E_k >= \frac{h\omega}{e^{h\omega/kT} - 1} \tag{11}$$

(note that the exponent of the exponential now is positive and not negative as usual!). This formula is what we have to substitute to $< E_k >= kT$ in eq. 4, it goes down very fast for higher frequency. We obtain a curve that fits perfectly experimental data:

$$I(\omega) = \frac{\omega^2 < E_k >}{\pi^2 c^2} = \frac{h\omega^3}{\pi^2 c^2 (e^{h\omega/kT} - 1)} \tag{12}$$

This equation grows initially with ω as before, but at higher frequencies the exponential wins and everything goes to zero as it should be, the *UV catastrophe* was finally solved! This was the first *quantum* equation ever, it became very famous as the *Planck radiation law*, or Planck's blackbody equation. The problem of the ultraviolet emission of hot body of equation 4 was solved for ever and *quantum mechanics* was born.

The electron double-slit interference Experiment

This experiment was at first conceived partially as a *thought experiment*, or from a German word a *Gedanken* experiment. However, everything we will say about it is now a confirmend experimental fact.

Suppose we have an electron cannon. This is a machine that shoot electron, exactly like an old CRT screen, or like the electron source of an electron microscope. These electron, at first, they were considered to be particles of matter, so they must behave like that. What happens in the experiment is that if we make the electron pass through a doble slit and on the other side we place a fotographic plate, instead to have a localize pattern of the same shape of the slits, we observe a figure of interference... (!)

[FIG]

The conclusion appears to be absurd! How is possible that electrons behave like waves? The researchers then tried to shoot one electron by one, at big distance in time. When only one electron was shot on the double-slit, one little spot was visualized on the photografic plate. If few electron where shot, few little dots were observed. If many electrons were shot, one by one, many little dots appeared, but incredibly enough, the dots formed the shape of an inferference pattern again!

This made researchers think hard of what can be the cause of this. It was like the electron was interfering with himself, somehow. When the researchers tried to visualize which of the two slits it passed through, putting a detector near the slits, then something even more strange happened: the electron behaved again as a particle. No interference pattern, just dots aligned perfectly with the slit.

In conclusion, if the electron have the option to pass through slit one or slit two, it behave like somehow a wave, and we see an interference pattern on the screen. If we measure where the particle has passed through using a detector, we do not see any interference, simply the electron go straight on the screen, and we see the shape of the slit.

So electrons have a *dualistic* behaviour. This idea was firstly established by professor De Broglie. He said that there is a dualism on the behaviour of matter, that depending on conditions it behave like a particle or like a wave.

To formalize mathematically what was happening, we have to say that our experimental result is an interference pattern on our photografic plate. The intensity of the pattern is proportional to the number of particles that hit the plate. In other words it is proportional to the *probability* that a particle hit there in a given time. So our measurable parameter is not anymore a position of a particle, like in Newtonian physics, now we only have a *probability* P. Because the pattern formed by this probability is an interference pattern, we can associate to the particle a *probability wave*, or *wave function* to the particle. This wave can be written this way:

$$\Phi = e^{-i(\omega t - kx)} \tag{13}$$

like any other wave. We have no idea at this stage of the physical meaning of ω or k, or the time t, we just know that x is the space. If we do this, we can say that my particle can pass either through the slit one or slit two s_1 or s_2, and the final wave is the sum of the two waves:

$$\Phi_{12} = \Phi_1 + \Phi_2$$

Of course, the *sum* of two waves, produce an interference, so Φ_{12} has the shape of an interference pattern, please do not forget that this is a complex function that has the shape of a wave. Our experimental result is insteat a *real* value, the interference pattern we observe, that is the *module* of this interference wave, so we can write:

$$P_{12} = |\Phi_{12}|^2 = |\Phi_1 + \Phi_2|^2$$

The observation and the study on this experimental facts brought the researcher to astonishing conclusions that can be summarized in the so called *three principles of Quantum Mechanics*:

0) A particle has within itself a wave that is called *wave function* and generally expressed as the complex wave

$$\Phi = e^{-i(\omega t - kx)}$$

1) The *probability to find the particle* is expressed as the module of ϕ :

$$P = |\phi|^2$$

2) If a particle has two alternatives ways to reach a point in space x, the probability to find it has the shape of an interference pattern:

$$P_{12} = |\Phi_{12}|^2 = |\Phi_1 + \Phi_2|^2$$

3) If the particle has no alternatives (it has been *measured* where it has passed), then the probability to find the particle is not an interference, but the bare sum of two probabilities

$$P_{12} = P_1 + P_2 = |\Phi_1|^2 + |\Phi_2|^2$$

Please note that since Φ is defined as the complex wave in eq.(13), its module square is of course just a real number, and in ideal case it is just 1 !

De Broglie Hypothesis and Heisember principle

We have the experimental fact that electrons diffract exactly like waves, like light or like water waves. This is a fact, so researchers had to think a way to represent particles as wave. The idea is that particles have an *inner* probability wave called *wave function* Φ and that their probability to be found in a place is the square of this function. The *De Broglie Hypothesis* is that the energy of such a particle is given by $E = \frac{h}{2\pi}\omega$ and that is momentum by $\frac{h}{2\pi}k$, where $\omega = \frac{2\pi}{\tau}$ and $k = \frac{2\pi}{\lambda}$
Now if a interference pattern is created, what is the relation between position X and momentum of a particle? We can calculate

this directly from the diffraction equation. We use simply the diffraction triangle in figure [FIG] and find that, for small angles, ΔP is equal to $P_0 * \alpha$. From De Broglie Hypothesis, $P_0 = \hbar k$, so

$$\Delta P = \hbar k \alpha$$

. If this is just a diffraction problem, we can find immediately $\alpha = \frac{\lambda}{d}$ where d is the aperture. But the aperture is actually *how well we know the position of our particle*, so we can call d as Δx. If this is so we have

$$\alpha = \frac{\lambda}{\Delta x} \tag{14}$$

$$\Delta P = \hbar k \frac{\lambda}{\Delta X} \tag{15}$$

Knowing that $k = \frac{2\pi}{\lambda}$ we finally deduce the fundamental relation of Heisemberg principle

$$\Delta P * \Delta X = h$$

This simply states that the knowledge of a particle position limits the knowledge of particle speed (momentum), and viceversa. Remember that this definition is not related to particle physics. It is a relation that can be derived by wave physics only. The Heisemberg principle is valid for audio waves, sea waves or any other *real* wave too !

The Bound States, stationary waves!

We have the experimental fact that electrons diffract exactly like waves, like light or like water waves. If we assume that the relation of the *wave function* $\psi = e^{\omega t - kx}$ and the physical propertiesof a particle is $E = \hbar w$ and $p = \hbar k$, then, as we found above, the particles interfere and produce a behaviour in which $\Delta x \Delta p > h$, that is called also *Heinsenberg principle*.

How we can be sure that the *De Broglie Hypothesis* $E = \hbar w$ and $p = \hbar k$ is really correct ? After all, it looks really strange. A particle of a definite energy E, would have a *probability to be found* in a certain place as

$$P = |\psi|^2$$

that is simply $P = const.$, a value the same everwhere. In other words, if the particle can be found anywhere we do not know where it is; this sounds very very strange !

Now we consider an atom, where particles are not free, but confined (bound) around the nucleus of it. Electrons are to be found only in a certain place. If is true that there is a *wave function* associated with it, it must be a *stationary* wave, like the one of a guitar or a violin. If this is so, a mechanical analogous implies that the violine wave must resonate ONLY with fixed wavelength, the fundamental and all its *harmonics* (the *harmonics* are the frequencies multiples of a certain fundamental frequency f_o, that is $2f_o$, the second harmonic, $3f_o$ the third harmonics and so on). Then also in our atom, the probability to find the particle will be confined to fixed energies

$$E_n = e^{\omega_n t}$$

were w_n are multiples of a fundamental w_o: $w_n = \{w_o, 2w_o, 3w_o \ldots\}$. This is a characteristics of *bound states*, where the particle is confined somewhere, so there is no x dependence, and the wave function depends only on time.

Is there a way to *localize* a particle still using the *De Broglie Hypothesis*? What happens if we superimpose different frequencies on a wave? If we remember wave mathematics, we should realize that the sum of slightly different frequencies produce *beats*. Beats are waves modulated in amplitude. Beats are very well known to musicians. If we play two guitar strings tuned almost the same $f_1 \approx f_2$, easily we can hear the beats that have frequency centered about the difference between the two frequency $df = f_2 - f_1$.

More interestingly, if we add up more nearby frenquency, not just two as above, but many in a almost continuous way, we obtain a particular set of interference, generally called a *wave packet*. It is a wave distributed along many frequencies with a bump of amplitude localized around center frequency. To *localize* a particle, we have to consider that the wave function

$$\psi = e^i(wt - kx) \tag{16}$$

contains both a space and time dependence. If we fix the time t and consider only k, our *wave packet* will be composed by the sum of many waves of different *wave number*, instead of frequency, but the mathematics will be exactly the same. So, because the wave function represent the *probability to find the particle*, the particle is localized at the center of the wave packet! This means that a particle is represented by the superposition of many wave functions (16) with similar, but different wave numbers. Moreover, if we shorten the difference in wave number, we obtain a wider localization and viceversa. Because the wave number represent the momentum of the particle we have again the situation described in the Heisemberg principle, a sort of $\Delta P \Delta X > const$...! If we use the definitions of energy and wave packet as before, we will prove this fact easily again. See figure 2.

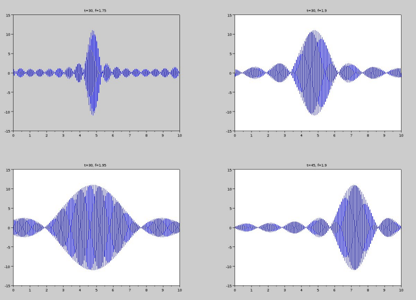

Fig. 2. The superimposition of several waves with similar wave number k. If we increase the width of the wave number span (we increase ΔP in Quantum Mechanical analogous) we have a better localization, as Heisemberg principle should indicate. Also, if we increase time (lower panel on on the right), the *wave packet* moves right, the analogous of a particle moving in space toward the right.

The Dirac representation

Now we know that what we thoght it was a particle, an electron or a photon, are not corpuscole, but they behave like waves, so they *contain* wave functions within themselves. We can write this wave function like this: $\psi = e^{-i(\omega t - kx)}$. Also we learned from Planck black-body equation, the Bohr atom, Einstein photoelectric effect and other experiments that in this equation the parameter ω has the physical meaning of Energy and the parameter k is the momentum. The *De Broglie* hypotesis is $E = h\omega$ and $p = hk$. Also, we have learned that the *probability to find a particle* is simply given by

$$P = |\psi|^2$$

This implies that a moving particle is represented by a *wave packet* where many waves of different energies (momentum and kinetic energy are related) overlap together, instead a steady particle is *bound* in a place and must have only fixed falues of energy $E = h\omega_n$ like a resonanting violin string. Now that we established these things we come back to the original *double slit problem* we discussed above. Everything is expressed mathematically in terms of probability, not enymore in position as in classical mechanics. How we can develop a simpler mathematical framework to calculate these probabilities? One way was introduced by prof. Dirac and still used today.

Suppose we indicate the position of a particle in one place, in our formulation we can call it like this $e^{-i(\omega t - kx)}$, to make it a little bit smaller we use this indication: $|\psi >= e^{-i(\omega t - kx)}$. What happens if two of these *wave functions* interfere? The result depend in how many dimensions we consider the problem. In one single dimension x, we will have *beats*, the probability to find the particle $|\psi|^2$ will be a figure of interference, as already discussed above. However, to reproduce the infamous *two* *slits electron experiment* we must proceed in two dimensions, we need two space variables x and y and two wave numbers k_x and k_y. How we can write mathematically the interference of two two dimensional waves? We do not go in details, but take in account that for each point in x, we need to *integrate* (sum up) the effects of all waves coming from differents y. So the mathematics is still conceptually the same, but heavier to write and calculate. Dirac representation help us to simplify. Lets consider that our waves are complex vectors, so the result of the sum of two of them is something like this:

$$e^{\vec{A}\cdot\vec{B}}$$

If we use the De Broglie hypothesis this will be of the form:

$$e^{-i(\vec{p}\vec{r}_{12})}$$

where r_{12} is the vectorial difference between position x_1 and x_2. Dirac introduced this notation: $< \psi_1|\psi_2 >= e^{-i(\vec{p}\vec{r}_{12})}$ we intentianolly ignored the presence of an integral here. In this way we can express very compactly the probability to find the particle if has moved from one place to another. Equivalence

- a method to represent the physics of particles in QM without writing all the waves - the example of slit problem. - an example with multiple levels slits

The equivalence with vector methematics

- the similarity with decomposition in *base states* to the projection of a vector in its *base coordinates.* - the physical meaning of base states: they represent alternative, mutually exclusive states

The Hamiltonian Matrix

- the amplitude of transition from $\bar{r_1}$ to $\bar{r_2}$ is

$$< r_1|r_2 >= e^{\bar{p}\bar{r}_{12}}$$

- The definition of *operator*: $\langle\chi|a|s\rangle$ - how the operators changes in time:

$$\psi(t+dt)\rangle = U(t+dt,t)\psi(t)\rangle \tag{17}$$
$$\langle j|\psi(t+dt)\rangle = \langle j|U(t+dt,t)|\psi(t)\rangle \tag{18}$$
$$\langle j|\psi(t+dt)\rangle = \Sigma_i\langle j|U(t+dt,t)|i\rangle\langle i|\psi(t)\rangle \tag{19}$$
$$U_{ij}(t+dt,t) = \langle j|U(t+dt,t)|i\rangle \tag{20}$$
$$C_{ij}(t) = \langle i|\psi(t)\rangle \tag{21}$$
$$C_j(t+dt) = \Sigma_i U_{ij}(t+dt,t)C_i(t) \tag{22}$$
$$U_{ij} = \delta_{ij} + a_{ij}\Delta t \tag{23}$$
$$C_j(t+dt) = \Sigma_i(\delta_{ij} + a_{ij}\Delta t)C_i(t) \tag{24}$$
$$C_j(t+dt) - C_j(t) = \Delta t\Sigma_i a_{ij}C_i(t) \tag{25}$$
$$\frac{C_j(t+\Delta t) - C_j(t)}{\Delta t} = \Sigma_i a_{ij}C_i(t) \tag{26}$$
$$\frac{C_j(t)}{dt} = \Sigma_i a_{ij}C_i(t) \tag{27}$$
$$i\hbar\frac{C_j(t)}{dt} = \Sigma_i H_{ij}C_i(t) \tag{28}$$

Propagation in a crystal lattice

- explain that it is normally difficoult to the electron to circulate in a solid crystal.
- cross section of electron 1 Amstrong
- cross section calculation:
- calculate the volume "shadow" behind the target *ball*

$$N_{int} = \quad n_{beam}V \tag{29}$$
$$N_{int} = \quad n_{beam}\pi R^2 vt \tag{30}$$
$$N_{intTime} = \quad n_{beam}\pi R^2 v \tag{31}$$
$$\sigma = \quad N_{intTime}/J_{beam} \tag{32}$$

where J is the *flux* defined as $J_{beam} = n_{beam}v$ and n_{beam} is the *beam density*, or the number of particle per unity of volume.

We can define another important parameter λ, that is called usually *mean free path.* It is the average length that the particle can run free. This parameter is as important as τ (the average time a particle runs free without collisions) and has almost the same meaning. The mean distance the gas particle can go -on average- before it experience a collision. Now let's try to relate some gas parameters that we know. Let's ask ourselves, what is the probability of collision after the particle has moved a distance dx ? We know the answer, this probability (for only *one particle*) is:

$$\frac{dx}{\lambda} \tag{33}$$

Why? Because if I am located in the middle of tables separated one meter each other and I move of one meter... I am sure -on average- that I will bump on a table. However, if I move only half a meter, on average, I have 50% probability to bump on a table. That's the simple linear relation expressed by 33. dx is how much I move among tables and λ is the distance between tables in our example. Now, lets consider it from another point of view. If we have a box of volume dV, with particle density n, what is the probability of collision in a small section of it of length dx ? Well, as we know the number of particles in this section is $nAdx$, where A is the area of this section (see figure 3).

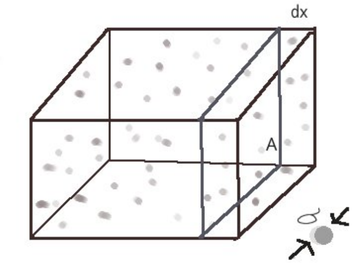

Fig. 3. A scheme for the modeling of the collision probability. The *cross section* is represented by the average area of a single gas molecule.

If the every single particle has an average area σ, then the total area occupied by the particle is $\sigma nAdx$. If we divide this area with the total area available (which of course is A), we obtain the probability of collision within this section of length dx: σndx. But this value must be equal to eq.33, so finally we have:

$$\frac{dx}{\lambda} = \sigma ndx \tag{34}$$

simplifying this yields this very important relation:

$$\lambda = \frac{1}{\sigma n} \tag{35}$$

this equation is very important because it relate the particle density, their *cross section* σ and their *mean free path* in a particle system each other with a very simple and compact formula.

A semiconductor device: PN junctions

We studied how the energy that a particle has, in quantum mechanics formalism, is represented by the parameter E in the equation:

$$\psi = e^{-\imath(wt-kx)} = e^{-\imath(\frac{E}{\hbar}t-\frac{p}{\hbar}x)} \tag{36}$$

because we define the energy $E = \hbar\omega$ and the momentum $p = \hbar k$. In the previous chapters we came to the conclusion that the probability amplitude of transition between states $|i\rangle$ and $|\psi\rangle$ that is $C_i = \langle i|\psi\rangle$ changes accordingly to the *Hamiltonian* equations studied above. As a consequence, if the parameter E represents the Energy of a particle that is adsorbed by an atom, this energy E must be contained between a range (a *band*) of values within

$$E = E_0 \pm 2A\cos(bk)$$

where E_0 is an arbitrary base energy reference, A is the energy necessary for the particle to *leak* from one atom to the adjacent, and b is the distance between them. As we have seen, the very same conclusions can be reached if we represent a particle that leaves an atom, not one that is absorbed by one. So we have two energy bands, one for the particles absorbed by an atom, one for those that leave it. These two allowed bands are usually called the electron band and the hole band because in the most common situation the particle studied is an electron, and a missing electron condition is called a *hole*.

The meaning of the bands is that any particle that does not have enough energy to be within the band, cannot exist. So, we can say that there is an *Energy gap* between the hole band and the electron band. Where do particles gets their energy? In absence of anything else of course by thermal energy (!)
So, because of thermal Energy, we expect to have a certain number of electrons and holes in their band in a certain distribution

in function of temperature. The most natural distribution is the *Boltzmann* distribution

$$N_e = N_{oe} e^{-E_e/kT} \tag{37}$$

$$N_h = N_{oh} e^{+E_h/kT} \tag{38}$$

$$N_e N_h = const * e^{Eg/kT} \tag{39}$$

$$\tag{40}$$

where we have multiplied the first two to obtain the third equation, naturally $E_g = \Delta E = (E_e - E_k)$. From this last equation, we understand that if the temperature increases, we put more electrons or holes in the band, so we have more carriers for possible conduction of electricity.

Suppose now that in a crystal of a certain atomic species, we introduce a different atom with different valence. If we do so, we are able to introduce a possible hole or a possible electron for the conduction bands. Then a material with many impurities that introduce a hole, will have an energy band lower than a meterial with impurities that introduce electrons. The question is: what will happen I put in contact these two materials? We form a so called *junction* where the potential will change along the crystal axis x that runs along the direction orthogonal to it.
We have to consider that Energy potential is related to electric potential by the simple relation $E = qV$, where V is the voltage (difference of potential).

Near the interface between the two material, the juction, we will have a slope of potential, so a diffusion process will begin. Lets consider only ONE type of carriers here, for example the "p" carriers. The more "p" carriers in one the "P" side, want to diffuse and migrate to the other side of the crystal. However, the ratio of carriers that will actually reach the "N" side will depend on the energy barrier in the junction accordingly to the usual Boltzmann distribution. So at the thermal equilibrium:

$$\frac{N_p(N - side)}{N_p(P - side)} = e^{-qV/kT} \tag{41}$$

where with P and N we indicate the two doping and majority carriers of the material. Notice also that qV is the energy required to carry a charge q through a potential difference V. What is the physical meaning of this equation? This means that carriers will diffuse from P-side to N-side because of their inherent thermal energy, but only the fraction that has enough energy qV will reach the other side. Please notice very well, that also the opposite phenomena will occur: P carriers in the N-side, will try to migrate to the P-side... this is a current in the opposite direction. In thermal equilibrium, we expect that these two equal to zero! The absolute value can be called I_0 and is equal to:

$$I_0 \approx N_p(N - side) = N_p(P - side) e^{-qV/kT} \tag{42}$$

So I_0 is a *diffusion* p-type carrier current running from left to right and from right to left within the Junction, just for reason of thermal carrier diffusion. If we apply an external potential difference $-\Delta V$ to the junction, what will happen? The potential will be no longer V, but become $V - \Delta V$. So the current of positive carriers running in the junction from P-side to N-side will be:

$$I_1 \approx N_p(N - side) = N_p(P - side) e^{-q(V-\Delta V)/kT} \tag{43}$$

This current is from P-side to N-side and it is bigger than I_0 by a factor ΔV, so the ratio between the two is:

$$\frac{I_1}{I_0} = e^{+q\Delta V/kT} \tag{44}$$

or

$$I_1 = I_0 e^{+q\Delta V/kT} \tag{45}$$

it increases exponentially by external variation of potential ΔV. What about the current due to Np carriers in the opposite side, the N-side? The potential ΔV cannot change exponentially these carriers that are residing on the N-side! Why ? Because a positive carrier on the N-side sees a big potential slope V and goes straight on the other side, almost indipendently of ΔV (ΔV is of course considered to be much smaller than the junction potential V).

So we have the sum of two Np currents. One is due to carrier originated in the p-side. These are majority carriers and as we said increase exponentially with ΔV. The others are Np carriers originated in the N-side, these are minority carriers and even if the cross to P side, they encounter a positive slope, so they all reach P side without change. If ΔV is small compared to the junction V potential, the value of this current is always I_0. Summing up these two contributions and taking in account that they run in opposite directions:

$$I = I_0(e^{q\Delta V/kT} - 1)$$

if we plot this current I in function of ΔV we obtain the typical curve of a *rectifier*. The first electronic device was born: the Diode !