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From chance to the physical laws: Toy models to connect the microscopic and macroscopic understanding of physical phenomena

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Summary. — We propose an educational approach which is useful to present different physical phenomena that can be explained with microscopic and stochastic models and that are often explored by students with simulations based on the launch of dices. The discussion of the physical principles that rule the phenomena proceeds through a recurrent comparison between the results they obtained with the simulated models and the results of real experiments. The teaching proposal allows students to compare the experimental data obtained with analytical results and simulations. The effectiveness of our approach has been tested both with groups of university students and with a group of teachers.

1. – Introduction

Since ancient times men have tried to study and understand nature and the phenomena that characterize the world around them. This research, from the beginning, has taken different directions: that of the sky and the immensely large bodies, and that of matter, *i.e.*, the elements which build the sensible world, the extremely small. So from the earliest times men have questioned the nature of matter. These lines of research were originally mainly speculative, with hypotheses that, today, we would hesitate to define scientific, and the ancient theories seem to be, sometimes, bizarre when viewed by the physicists of the third millennium. However, great questions about nature were answered in the philosophical essence since the beginning of Western culture and, conversely, many questions remain matter of speculation even though our knowledge of nature is now deeper. In Ancient Greece, the battle was between the idea of a continuous matter and the idea of a world made of indivisible elementary particles, the atoms. More generally, following the reasoning of the ancient Greek philosophers, at least three of the fundamental dichotomies of physics were clearly considered: Continuous-Discrete, Macroscopic-Microscopic, Random-Causal. So, beyond the theories of nature, which today may seem naive and imbued with poetic aspects, beyond the methods of investigation, based more on refined logical reasoning than on a real observation of reality, ancient philosophers had already the essence of a central and very current juxtaposition: the conflict between a macroscopic world, continuous and ruled by deterministic laws, and a discrete microscopic world ruled by the laws of randomness. Modern science has only partially solved this conflict and some great scientists have rejected, and some others today reject, the idea of a world governed by randomness. In fact the advent of quantum mechanics in the early 20th century and the formulation of the Heisenberg uncertainty principle saw the end of the classical way of thinking among physicists regarding the determinacy of nature.

In this paper, we will report the results of some activities that our research team has designed to stimulate, in students, the construction of a conceptual bridge between the microscopic world, ruled by randomness, and the deterministic macroscopic laws. We introduce this rapid overview of activities proposing a brief historical reconstruction discussing how a corpuscular view of matter has been established over the centuries and how the multiplicity of microscopic entities has often been considered as ruled by the laws of randomness.

Then we discuss an educational approach to some different physical phenomena that can be explained by means of microscopic toy models. Many of these models are stochastic and explored by students with rolling dices [1]. The discussion of the physical principles governing the phenomena proceeds through a recurrent comparison between the outcomes obtained with the models, the results of real experiments and simulations.

In fig. 1 we summarize the approach:

- The students' activity starts from a real experiment, which students can make in a laboratory by themselves by using simple and inexpensive apparatuses. This experiment can be supported or replaced by a simulated experiment. Data analysis allows the discovery of phenomenological macroscopic laws able to interpret the experiment.

- A model, which highlights the microscopic basis of the measured phenomenon, is introduced and students explore it and they obtain some data. In many cases this toy model is based on dices, it goes on by considering the problem in statistical and probabilistic terms, and allows students to compare the experimental data they obtain to both analytical results and simulations.

- The discussion of the physical principles governing the phenomena proceeds through a recurrent comparison between the outcomes obtained with the toy models and the results of real experiments.

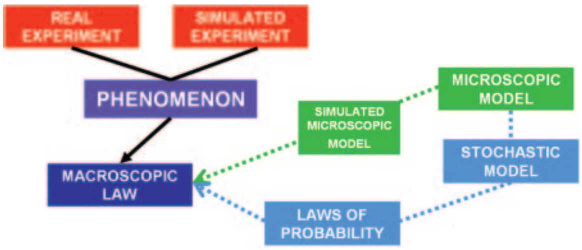

Fig. 1. – Diagram of the approach applied to each step of the sequence.

2. – Atoms, corpuscles and chance

The contrast between continuous matter and atomistic theory first started in Ancient Greece. Usually scholars report that the battle between continuity and atomism started from the Eleatics, a pre-Socratic school of philosophy founded by Parmenides in the early fifth century BC in the ancient town of Elea. Parmenides made the ontological argument against nothingness, essentially denying the possible existence of a void, while Zeno argued against plurality, space and the movement. These concepts were condemned by the Eleats as deceptive appearances. Zeno arguments are perhaps the first examples of a method of proof called *reductio ad absurdum* and each paradox is grounded on the idea of a continuous space and a continous time [2]. Some scholars [3] argued that Zeno of Elea's arguments about divisibility were formulated in response to the early Pythagoreans. However the majority of scholars assert that it came as a response to Parmenidean arguments [4-6].

Leucippus and Democritus (5th–4th centuries BC) "developed systems that made change possible by showing that it does not require that something should come to be from nothing" [2]. These ancient atomists theorized that the two fundamental and oppositely characterized constituents of the natural world are indivisible bodies, atoms, and void. The latter is described simply as nothing, or the negation of full. This reply to Parmenide's presumed that there are multiple unchanging material principles, which persist and merely rearrange themselves to form the changing world of appearances. According to Leucippus and Democritus, these unchanging material principles are indivisible particles [4].

The thought of Democritus met soon an illustrious opponent, Plato (427–347 BC). In fact also when he presented in *Timaeus* [7, 8] a physical theory based on indivisibles, Plato rejected mechanistic materialism and the idea of material atoms. In Plato's theory the four different basic kinds of matter —earth, air, fire, and water— are regular solids composed of plane figures: isosceles and scalene right-angled triangles. Because the same triangles can combine into different regular solids, the theory thus explains how some of the elements can transform into one another, as was widely believed. In this theory, the elemental triangles composing the solids are regarded as indivisible, not the solids themselves. Quite to the opposite, Aristotle asserted that the elements of fire, air, earth and water were not made of atoms, but they were continuous. Aristotle considered the existence of a void, which was required by atomic theories, to violate physical principles [9]. Thus atomism did not gain pre-eminence in the ancient world even if, after Aristotle, Epicurus and his disciples gave new life to the atomistic doctrines.

In summary with ancient atomists the idea of a discrete microscopic world, made of atoms, was affirmed. But even within atomists, conflicting opinions emerged over the centuries. According to some scholars, the most interesting dichotomy concerned the deterministic behaviour of atoms, advocated by Democritus, set against the random motion of atoms(1) proposed by Epicurus (4th–3rd centuries BC), who attributed to the elements a spontaneous deviation (*clinamen*) from vertical motion. "Hence, this much is historically certain: Democritus makes use of necessity, Epicurus of chance. And each of them rejects the opposite view with polemical irritation. The principal consequence of this difference appears in the way individual physical phenomena are explained. Necessity

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(1) Most modern scholars [10-17] have argued that the random movement of the atom, namely the swerve (*clinamen*), was introduced by Epicurus in order to allow for human free will.

appears in finite nature as relative necessity, as determinism. Relative necessity can only be deduced from real possibility, *i.e.*, it is a network of conditions, reasons, causes, etc., by means of which this necessity reveals itself. Real possibility is the explication of relative necessity" [18]. Behind this contrast lies the need for Epicurus and Lucretius to eliminate any intervention of metaphysics to explain the behaviour of the natural world by introducing the concept of "chance", $\tau\upsilon\chi\eta$. With the epicureans the idea of chance enters the history of culture related to a mechanistic, materialistic and atheistic concept, which will be unacceptable in the Christian Europe of the Middle Ages, when Aristotlean ideas were pre-eminent. It follows that for many centuries atomism was abandoned. Only in the sixteenth and seventeenth centuries some philosophers resumed the atomistic and mechanistic themes. It was predominantly a "Christianized" and "devoted" atomism and mechanism, which placed as foundations of all of God's creation [19].

In the 16th century the atomistic doctrine was supported by Giordano Bruno, who, in his theory of minima, studied solid bodies as groups of atoms. Bruno's elemental theory refuted outright the dominant Aristotelian view by which the universe was finite but infinitely divisible, while Bruno rejected the existence of void, the material nature of atoms and mechanism. According to Bruno, atoms were incorporeal spheres with spatial locations. Soul, working through the intermediary of ether or spirit, joined these incorporeal, identical spheres to make a body.

In the history of atomism, the 17th century occupies a special place for two reasons: it saw the revival of Democritean atomism, and it saw the beginning of a scientific atomic theory. Galileo Galilei (1564–1642) in "Il Saggiatore" [20] discussed a complete physical system based on a corpuscular theory of matter, in which almost all phenomena are produced by "matter in motion". Descartes (1596–1650), one of the founders of modern mechanistic philosophy, did not accept atomism and proposed a "mechanical" philosophy of corpuscularism, which considered fullness and denied void [21]. Pierre Gassendi (1592–1655), the main supporter of atomism of his age, set out to "purify" epicurean atomism from its heretical and atheistic philosophical conclusions [19]. During the 17th century, Europe experienced a series of changes in thought, knowledge and beliefs that affected society and produced a cultural transformation. It was a revolution of the mind, a desire to know how nature worked, to understand the natural laws. The advances in knowledge resulted in a powerful wave that, emerging from astronomy and mathematics, swept the habits, the culture, and the social behaviour of an era.

While the atomic theories of Democritus had been pure speculations, incapable of being put to any experimental test, scientists of the modern age needed a modern scientific atomism. Thus the concept according to which matter consists of small and invisible fast-moving atoms was taken up again in the seventeenth century and used to explain various phenomena, in particular, the properties of gases. In this case, from a pre-scientific idea produced by philosophers who tried to reconstruct an image of the world, atomism becomes a scientific theory which allowed to build models able to quantitatively explain the observed macroscopic phenomena. First Robert Boyle (1627–1691) emphasized that the "air is elastic", experimentally discovered the law that bears his name and tried to interpret it using a microscopic model. On this basis, the first quantitative formulation of the kinetic theory of gases was developed in 1738 by the Swiss mathematical physicist Daniel Bernoulli (1700–1782). Bernoulli's theory introduced the idea that temperature could be identified with the kinetic energy of particles of an ideal gas [22].

At the beginning of the 19th century the idea of an atom as a physical entity made its way thanks to the contribution of John Dalton (1766–1844), the founder of the modern theory of the chemical atom, and Amedeo Avogadro (1776–1856), the first to give its current form to the theory of the chemical atom.

Thus the atomistic model was developed during the nineteenth century and some pioneers of the kinetic theory (which were neglected by their contemporaries) were Mikhail Lomonosov, Georges-Louis Le Sage, John Herapath and John James Waterston [22, 23]. In 1856, August Kronig (probably after reading a paper of Waterston) created a simple gas-kinetic model, which only considered the translational motion of the particles. Kronig had paved the way with his article, and the first scientist able to overcome the widespread reluctance to seriously consider the kinetic theory was the German physicist Rudolf Clausius (1822–1888) [22].

In this developmental phase the kinetic theory did not necessitate the introduction of either the probabilistic concepts or the statistical method introduced by Clausius after a couple of years in the derivation of the formula of the mean free path. Subsequently, Maxwell transformed the kinetic theory of gases in a fully statistical doctrine. It seems in fact that, at least up to Maxwell, the physicists of the nineteenth century had always assumed that gas was a deterministic mechanical system. It follows that if the superior intelligence imagined by Laplace had possessed all the necessary information about the state of motion of all the atoms at a given instant, he could have calculated their positions and their velocities for each other instant, deriving the macroscopic properties at the same time.

So with Maxwell and Boltzmann, in the studies concerning entropy, the second principle and irreversibility, chance and the laws of probability become the pillars on which to build a bridge between the microscopic world of molecules and the macroscopic world of the laws of gas [22]. In the twentieth century, thanks to the birth of Quantum Physics, the idea of discretization extended from matter to electromagnetic radiation and to physical quantities, such as energy or angular momentum. Also here it becomes necessary to build a bridge between macroscopic phenomena (for example, the absorption of a ray of light that passes through a material) and microscopic objects, molecules and photons. But in this case the classical laws of probability only partially help us fill the distance between the macroscopic world and the microscopic world, governed by a new probability with laws different from the classical ones. In the world of classical phenomena in which probability is epistemic, one has to deal with conclusions that are expressed probabilistically because of our ignorance of the real state of the system under examination, and the classical laws of probability apply. Quantum physics introduces a new concept of probability, *i.e.*, a probabilistic description of events that cannot be attributed to ignorance and requires the application of the laws of quantum probability [24].

3. – Microscopic models without randomness: The gas laws

Following the track of the historical development we start with a simple and traditional activity about Boyle's law, with the aim of allowing a comparison between the results of a toy model and the outcomes of a real experiment The experiment is aimed at verifying Boyle's law for isothermal transformations and the macroscopic concept of pressure with the use a graduated syringe and weights. In this experiment, weights are stacked on the platform on top of the syringe and the gas volume inside the syringe is measured using the syringe's scale. The additional pressure placed on the syringe can be calculated by adding atmospheric pressure to the force per unit area the weight and the platform put on the syringe. Results are in agreement with the Boyle's law, pV = const. (see fig. 2). The experiment can go with a simulated experiment [25] reproducing the same

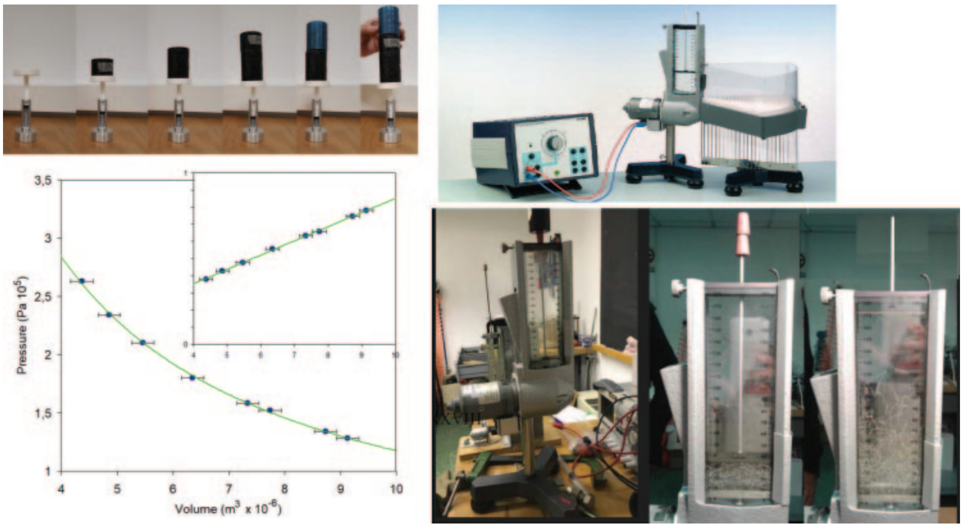

Fig. 2. – (Left) The syringe is plugged so that air is unable to escape while weights are being piled on. The platform makes it easier to balance the weights on top of the syringe. Adding weights to the syringe increases the pressure. Thus the measured pressure *vs.* volume and the linear dependence of the inverse of pressure are shown. (Right) Kinetic gas theory apparatus. By means of the model apparatus for kinetic theory of gases, the motion of gas molecules is simulated and Boyle's law is obtained.

phenomenon. Thus the volume can be measured as a function of pressure. A second activity is aimed at illustrating the microscopic interpretation of this phenomenon in terms of average momentum transfer from the gas molecules to the recipient's walls with the use of the *Kinetic gas theory apparatus*(^{2}) (fig. 2, right) consisting of a chamber with a piston sustained by the agitation of tiny balls put into motion from the vibration of the underlying bottom floor. Also in this case students can carry out measurements of the volume as a function of pressure (added weights on the top of the piston) while the chamber filled with balls can be explained using the applet "Gas Properties" [26]. Thanks to the use of this analogy and the use of the "PhET" applet, students can build themselves a microscopic image of the gas.

To derive the laws of gas quantitatively starting from the kinetic theory, we could use the approach reported by many textbooks. In the construction of the bridge between the macroscopic phenomenon and its microscopic explanation, it is not initially necessary to introduce any stochastic element. Thus it is possible to use a model with a single particle in a box, moving backwards and forwards along a straight line with constant speed. For the particle in a box and, more in general, for one-dimensional (mechanical) systems consisting of a particle constrained by a potential well having a single minimum (sometimes called a U-shaped potential) there is an analogy with thermodynamics [27-31] defined by the correspondence between mechanical and thermodynamic variables: total mechanical energy, U_T, as the analogue of internal energy; force on the particle averaged on one period of the particle orbit within the well as the analogue of pressure, p_T; the kinetic energy of the particle averaged on one period divided by the Boltzmann

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(^{2}) `https://www.phywe.com/en/kinetic-gas-theory-apparatus.html`.

constant, k_B, as the analogue of temperature, T_T; and the half-length of the periodic orbit as the analogue of volume, V_T. In this way one can derive an "equation of state" of the general form

$$p_T V_T = k_B T_T. \tag{1}$$

This analogy is sometimes useful in the educational practice, for example, for providing an intuitive picture of phase transitions: by considering the two motion regimes of a simple pendulum or similar system, *i.e.*, oscillatory up to a threshold value of the total energy, and then rotational, one can find the analogue of a solid-gas phase transition, going as far as computing the analogues of specific heat, critical parameter and so on [29, 31]. In fact, a mechanical analogue of entropy preserving most of its properties can also be found [32]: this quantity, known as the Helmholtz entropy S_H, is the logarithm of the phase space volume enclosed by the curve of constant energy, while the particle moves back and forth between the two turning points in the potential,

$$S_H = k_B \ln\left(\frac{1}{h}\oint p\mathrm{d}x\right), \tag{2}$$

and h is a constant with the dimensions of action which, formally, serves the purpose of making the argument of the logarithm a pure number.

The fact that an entropy function, preserving most of the properties of the Boltzmann entropy and essentially equivalent to it for macroscopic classical systems, can be constructed even for a one-dimensional mechanical system may suggest the idea that randomness is not an essential ingredient for understanding the second principle of thermodynamics. This has also been argued, from a different perspective, by the proponents of the *typicality* approach to the foundations of statistical mechanics [33]. However, we believe this not to be the case.

In fact, both the Helmholtz and the Boltzmann definitions of entropy require the introduction of a quantum of action, h. Formally, this can be thought of as needed to make the argument of the logarithm non-dimensional but, physically, it represents a necessary assumption to prevent the entropy from diverging at zero temperature, in contrast with the third law of thermodynamics.

In summary, the toy model and the following reasoning show how the initial development of kinetic theory does not need any assumption of randomness. However, when entropy comes into play, the issue becomes more complicated since the mathematical and physical meanings of entropy both seem to require a coarse grained discretization of phase space. And since this is naturally done by taking into account the uncertainty principle of quantum theory, it is in this way that chance comes to play a central role.

The activities discussed in this section were used with the students to recall the main concepts of the kinetic theory of gases and show how the latter theory does not require introduction of any stochastic concept. Thus the concept of entropy was critically introduced, showing the intrinsic need to introduce some form of indeterminacy into the theory.

4. – Microscopic stochastic models: The thermal equilibrium

The second activity is aimed to explore the thermal equilibrium and to ground it on a microscopic basis. Students started by performing a simple experiment. In this experiment students, using temperature sensors, measured the time evolution of two bodies in thermal contact. The experiment, which can be simulated thanks to a software as Energy2D [34], was carried out using a dewar filled with water at room temperature and a small metal cylinder, immersed in the dewar water, in which students poured a small quantity of water at much higher temperature [1]. The corresponding toy model is based on a board with two rows of different length of numbered squares; on each square of the row one coin (at most) can be placed. Bodies in thermal contact are represented by rows of squares on a cardboard table, which exchange coins placed on the squares based on the roll of two dices. From the model, students can deduce the exponential approach to equilibrium (see figs. 3 and 4), the determination of the equilibrium temperature and the interpretation of the equilibrium state as the most probable macrostate. After the game, students use the probabilistic and statistic laws for bridging microscopic and macroscopic understanding of the heat transfer and equilibrium law. At the end of the activities concerning thermal equilibrium, based on both an experimental approach and a theoretical elaboration, students were able to answer some questions which summarise the content of the sequence:

- Is there a macrostate of equilibrium for the system? Which one? Why?
- What is the role of probability? How can the probability of a macrostate be computed?
- What do coins correspond to in the analogy between two bodies in thermal contact and the toy model game?
- Which physical principles can be obtained from the comparison between the toy model and the experimental data of the physical process of approach to thermal equilibrium?
- Which thermodynamic quantity is connected to the probability of a macrostate?

Furthermore the examples discussed showed the students that the description provided by thermodynamics is an intrinsically probabilistic one, and that macroscopic laws, such as the law of heat transfer, are based on microscopic phenomena which we interpret using a statistical description.

5. – Quantum particles and classical probability: The light attenuation

In fig. 5 we summarize the approach to the light attenuation following the diagram reported in fig. 1. Firstly we showed the phenomenon of light attenuation to the students with a spotlight (light is produced by quasi-monochromatic LEDs) and a small transparent container filled by liquid soap. The students easily noticed, observing the scattered light, both the scattering phenomenon and the attenuation of the incident beam. Then a quantitative experiment is performed. In this experiment students use a smartphone-based apparatus as a tool for investigating the optical absorption of a material and to obtain the exponential decay predicted by Beer's law [35]. The light from a LED goes through the liquid soap in a glass put on a black cardboard with a window. The ambient light sensor of a smartphone measures the intensity while the thickness of the soap is increased with a graduate syringe. The intensity *vs.* thickness measured for different LEDs shows the typical exponential decay with a characteristic length strongly dependent on the wavelength (see the results of experiments in fig. 6). The same phenomenological

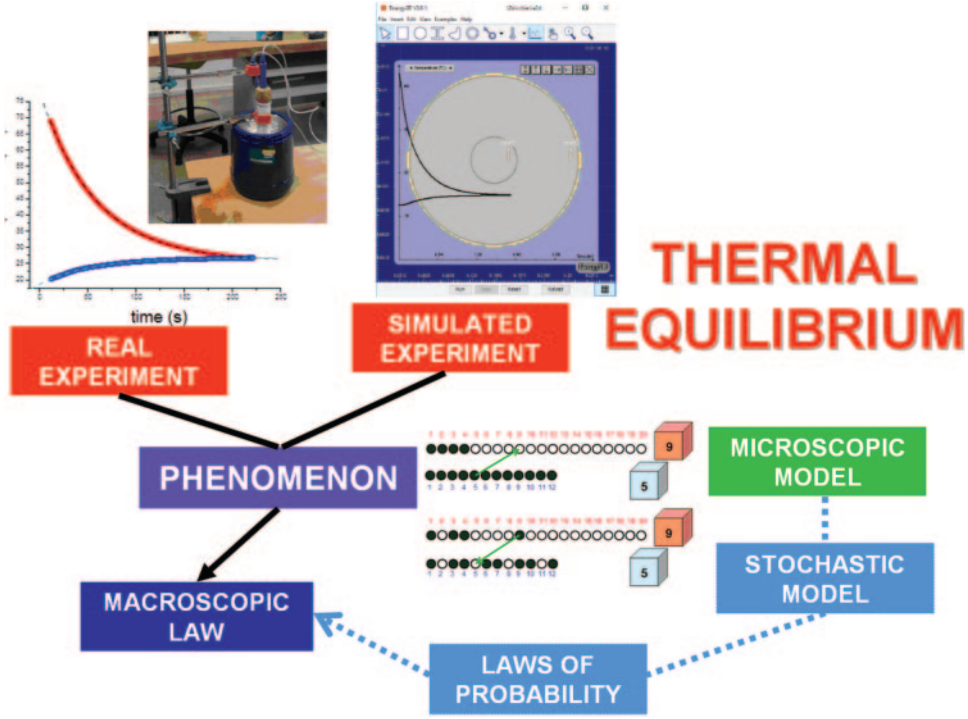

Fig. 3. – Diagram of the approach applied to the thermal equilibrium. In the top the experimental set-up and the results of the experiment and simulation.

law could be obtained by students by performing the simulated experiment [36]. Thus we present an educational approach to the Beer-Lambert attenuation law based on a stochastic toy model, in which incident photons are represented by rows of squares on a cardboard table and microscopic scatterers are placed at random according to the roll of a dice. In each square of the table an X, can be placed *i.e.*, microscopic scatterers are placed at random according to the roll of a dice. During the activity, students rolled the dice many times, each launch corresponding to a column, and inserted an X in the box

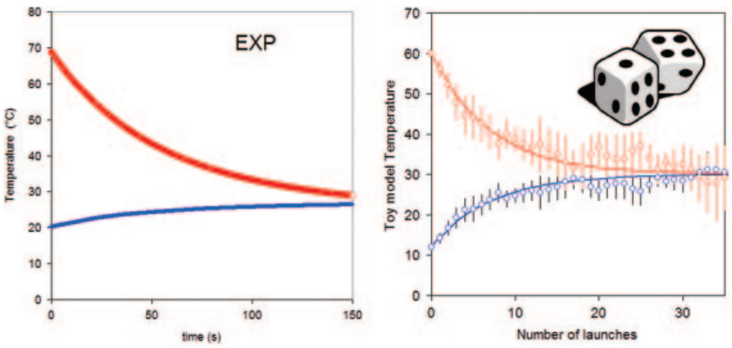

Fig. 4. – (Left) Results of the experiment about thermal equilibrium. (Right) Data obtained by students playing with the toy model.

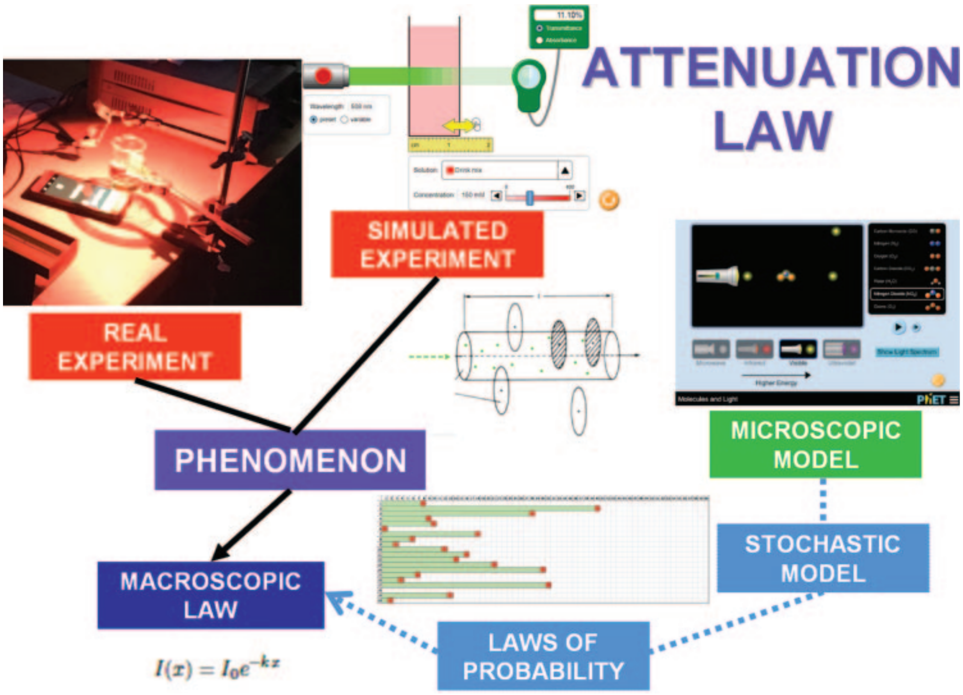

Fig. 5. – Diagram of the approach applied to the attenuation law. In the top left inset the experimental apparatus with the smartphone and the glass. The two simulations of PheT, The Beer' Law Lab (top middle) and Molecules and Light (top right) show the macroscopic and microscopic phenomenon of light adsorption.

corresponding to the line matching the extracted number. In this way they distributed the scatterers in a stochastic manner one by one. Finally they can infer from the simulation the exponential decay of transmitted light and the mean free path allowed to the simulated photons. Thus a corpuscular derivation of Beer's law is given emphasizing the stochastic laws which rule the microscopic world. With the aim of showing students how the matter-radiation interaction at different wavelengths is characterized, we have discussed with students the simulation "Molecules and Light" [37] which highlights the interaction processes between photons and microscopic components of matter.

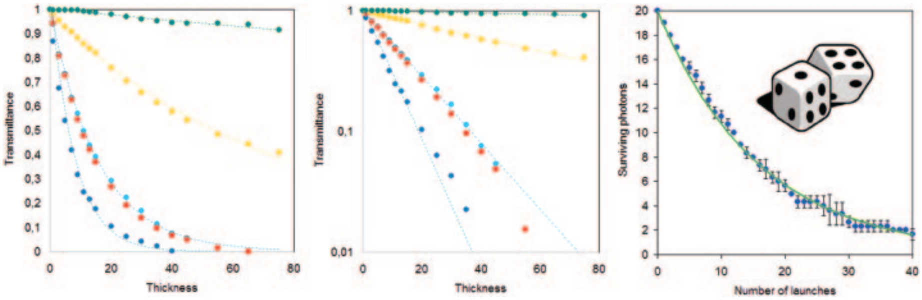

Fig. 6. – (Left and center) Results of the experiment about light attenuation. (Right) Data obtained by students playing with the toy model.

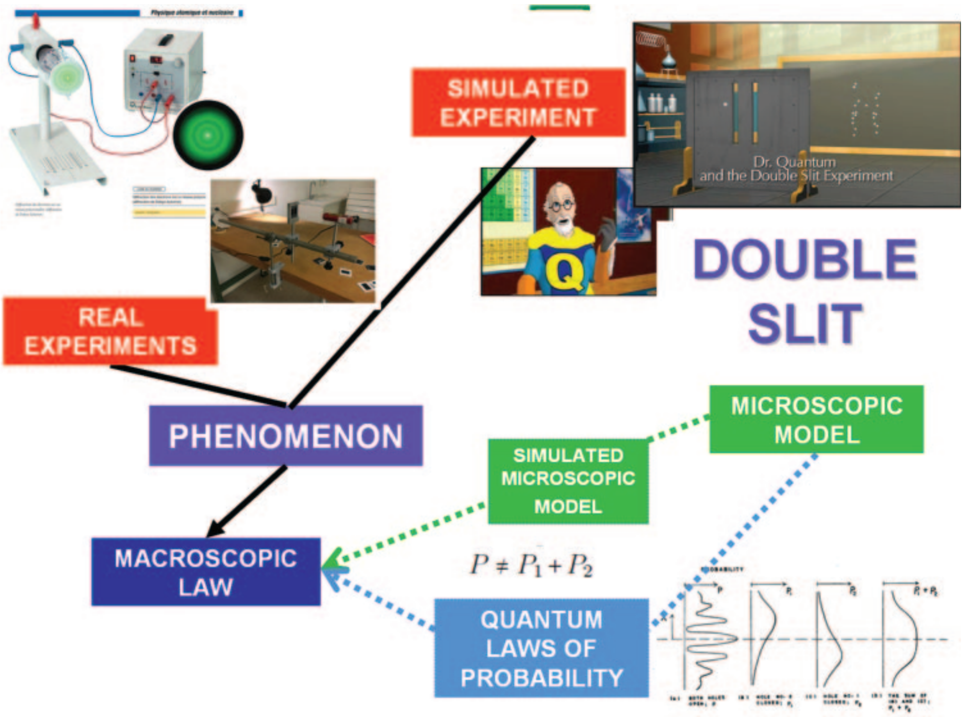

Fig. 7. – Diagram of the approach applied to the quantum model of light. In the upper left, the experiments: The electron diffraction experimental apparatus and the optical bench with a laser and a diaphragm with double slits. In the upper right a frame of the video where Dr. Quantum explains the double slit experiment.

After the game, students used the probabilistic and statistic laws for bridging microscopic and macroscopic understanding of the attenuation law, obtaining the exponential attenuation law and the mean free path. Thus a corpuscular derivation of Beer's law was given emphasizing the stochastic laws which rule the microscopic world. The discussion of the law in these terms is advantageous because it provides more physical insight than the common approaches and because it shows the capability of the corpuscular model of light in explaining such macroscopic phenomenon. However, the interactions are treated following the rules of classical probability.

6. – Quantum probability: The double slit interference

In fig. 7 we summarize the approach to the double slit interference following the diagram reported in fig. 1. In the study of the attenuation law, the behaviour that follows the laws of classical probability is attributed to the photon. So as long as we limit ourselves to studying phenomena such as absorption and transmission, no paradox seems to emerge and the basically macroscopic behaviour seems to be the fruit of classical probabilistic behaviour. The bizarre aspect of Quantum Physics manifests itself when the probability no longer applies to a set of particles but to the single particle with paradoxical consequences. It is the case of the single electron or single photon interference by double slit [39, 40]. Feynman originally outlined his thought experiment as a way of illustrating wave-particle duality in quantum mechanics. He invited to imagine firing individual electrons through two slits and then marking the position where each electron strikes a screen behind the slits. After many electrons have passed through the slits, the marks on the screen will comprise a diffraction pattern illustrating the wave-like behaviour of each electron. But if one were to cover up one of the slits so that each electron could only pass through the other slit, the diffraction pattern would not appear showing that each electron does indeed travel through both slits.

To introduce the concept of quantum probability we propose two real experiments, the first one about the double slit interference with a laser pointer, the second one about the electron diffraction from amorphous carbon [38]. In the commercial apparatus for electron diffraction, electrons emitted by thermionic emission from a heated filament inside the cathode are accelerated towards a graphite target by a potential difference. Then electrons arrive on a fluorescent screen where the interference frings can be observed and their positions can be measured to verify the De Broglie relation.

With the aim of presenting students with the behaviour of a single quantum object in a double slit experiment [39, 40] we showed a fragment of the video where *Dr. Quantum Explains Double Slit Experiment* [41]. The video displays the fundamentally probabilistic nature of quantum mechanical phenomena and also discusses how the detection of individual discrete impacts is observed to be inherently probabilistic, which is inexplicable using classical mechanics and the classical laws of probability. Thus we discuss with the students *The Concept of Probability in Quantum Mechanics* [24], *i.e.*, in the double slit experiment, the chance of arrival with both holes open is not the sum of the chance with just hole 1 open plus that with just hole 2 open.

7. – Conclusions

In this paper we presented a sequence of activities which stimulate students to reflect on the fundamental randomness of microscopic processes, one of the conceptually most relevant aspects of the modern physics. This sequence was tested with 60 university students at University of Trento during three years.

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