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Optical spectroscopy for biotechnology students

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Summary. — Spectroscopy is a fundamental and a professionalizing content for biotechnology students. In particular, optical spectroscopy represents an important link between physical optics, its main applications and its atomic-molecular interpretations. After a teaching intervention concerning physical optics, a laboratory-based activity, carried out with optical goniometer, was conducted with freshmen in biotechnology in the context of their physics course at Udine University (IT). The study aims to monitor students' reasoning and learning difficulties about the interpretation of discrete atomic spectra, so the activity was accompanied by a IBL tutorial and by a post-test inspired by the existing Physics Education Research literature. 56 students completed the tutorial, 45 of them competed the post-test. Here we report and discuss the results emerged from data analysis of the students' written answers.

1. – Introduction

Optical spectroscopy offers an important disciplinary contribute on the epistemological plan of physics, since it represents a conceptual bridge between classical and modern physics. It has an important applicative value in different fields: biomedical, astrophysical, social, conservation of cultural heritage and technological applications in general. It played a crucial role in the study of radiation emission leading to the construction of the quantized atomic model [1, 2], starting from Planck's quantum hypotesis [3], up to Balmer's series [4] interpretation due to Bohr [5]. Einstein's photon hypotesis in order to interpret photoelectric effect [6] paved the way in the searching of single-photon sources, while optical spectroscopy started to represent an interpretative referent and an investigation tool in semi-classical perspective.

On didactical plan its relevance regards cultural aspects, since absorption and emission of quantized electromagnetic radiation are fundamental concepts in physics and they represent some of the main investigative tools based on light-matter interaction. Optical spectroscopy, in particular, represents a context in which to understand the role of the

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energy in physics analysis, a validation modality of interpretative models through indirect measures and a way to interpret a code in order to get information on the changes and on the states of a physical system. Optical spectroscopy is therefore a methodological context in which the tools and methods of connection between experiment and theory in physics are prominent, since it allows to gain experience about the specific way of investigation in physics, offering the possibility to address the problem of understanding the Nature of Science (NOS) in operative terms [7-9]. Today optical spectroscopy is one of the main interpretative tool in the framework of the model in which, at microscopic level, structure of matter is quantized.

In Physics Education Research (PER) literature this topic is mainly addressed to learning difficulties related to specific contexts. An organic path in which optical spectroscopy is integrated as curricular contribution on interpretative plan is a recognized necessity. One of the main difficulties regards the association between spectral lines and energy levels [10] as well as the idea that every transition always takes place at the fundamental level [11-13], the interpretation according to which the emitted radiation is linked only to the final or initial level involved in a transition [13], or the idea that the number of distinct colors in a spectrum is equivalent to the number of energy levels [11]. The role of the fundamental level turned out to be controversial: researches have pointed out that it is not considered as an energy level [12], or the diffuse and persistent presence of the students' idea according to which it has zero energy [12,13], causing difficulty in assigning a meaning to negative energy values of the excited levels [12]. The Bohr model of the hydrogen atom is used in order to link the orbits with the levels, misinterpreting the symbolic representation of the orbit, performing trivial connection between spectral lines and the microscopic structure, assigning the energy value $E = h \cdot f$ to the level and/or the corresponding line, without mentioning the concept of photon [14]. Conceptual knots related to the energy quantization of the radiation concern the idea that a photon can be partially absorbed [13], or the idea according to which the atom must always make a transition between levels, although the energy of the photon does not allow it [13]. The idea that the radiation intensity is linked to the energy of the photons rather than their number has been found [15,13]. The need for microscopic models as interpretative instruments to overcome the conceptual knots of the systems behavior has been addressed by means of simulation tools [16, 17]. Also in introductory astronomy courses, where spectroscopy plays a key role in the interpretation of physical phenomena, there are difficulties related to the description of the light emission process by the atoms [18].

Conducted studies on this topic evidenced the persistent presence of students' spontaneous models concerning the formation of discrete spectra and their link with the discrete energy structure of an atom. These models have to be overcome in order to gain a scientific view of the topic [19,20] and develop formal thinking [21].

Within a research project based on the Model of Educational Reconstruction (MER) [22, 23] and carried out with Design-Based Research (DBR) methodologies [24-27], we decided to contribute in building a vertical path in which optical spectroscopy is an integrated part in estabilishing a bridge between classical and modern physics. In this perspective, we started the study from the conceptual knots recently outlined in the literature in the same laboratorial context described in [10-12]. We aim to build a vertical path for two main reasons: this topic needs to be introducted as a conceptual bridge between classical and modern physics, moreover there is a need for innovation of university teaching/learning (T/L) in life-science courses, whose importance is widely recognized [28-30]. Innovation of university T/L needs the students' personal involvement [31-33] in order to gain specific skills and promote students' conceptual change [34,35] with respect to the various courses also the introductory ones. The treatment of topics linking models knowledge and data that can be obtained with specific analyses is a fertile field for this purpose, and this is the case of optical spectroscopy.

In order to gain knowledge about students' reasonings concerning the elements linking experimental experience and the abstract models taught in physics and chemistry introductory courses, and to identify the main characteristics of the main conceptual knots, a laboratory-based study was conducted. The experimental activity allows students to observe and measure discrete atomic spectra in the optical band and it was integrated in a formative intervention module on optical diffraction, making use of a tutorial and a post-test. The experimental outcomes concerning students' reasonings are summarized in the following.

2. – Sample, context and reserch questions

The activity involved a group (N = 56) of freshmen in biotechnology, who passed the selection test among 200 applicants, from Udine University (IT) in the academic year 2015/16. They were attending a 3 CTS introductory physics course integrated with 10 hours of laboratory activities. The research described here was carried out in the framework of this specific course. Propedeutical issues concerning the activity (geometrical and physical optics, with special attention to optical diffraction in order to account for the characteristics of a light pattern caused by a diffraction grating, different kinds of light sources, discrete and continuous spectra highlighting the existence of a discrete energy structure in order to account for atomic spectra) have been treated in 6 hours. 2 hours were devoted to the laboratory activity with submitted tutorial, and 2 hours were devoted to the post-test. Before the laboratory, students attended an introductory chemistry course, dealing in particular with the following topics: atoms and molecules, the structure of the hydrogen atom, orbitals and quantum numbers.

In PER, a specif aspect is taken into account in the context of a wider thematic. In particular, in this research the aspect under investigation is the conceptual link between spectral lines and discrete energy levels in the context of optical spectroscopy. The present study aims to give answers to the following research questions:

- RQ1) Which role do students assign to the slit and to the diffraction grating in the experimental setup?
- RQ2) Which models are mainly used by students in order to describe the emission of light from an atom?
- RQ3) Which kind of reasonings and representations are used by students for the relationships between spectral lines and energy levels of the emitting systems?

3. – Methods and instruments

The proposed laboratory was based on the experiment of the optical goniometer (fig. 1). The goal was to measure the energies corresponding to the various emissions in the light from gas discharge lamps containing different elements (cadmium, helium, zinc, mercury). A short introductive lesson was given before the experimental activity in order to review the aforementioned topics, resumed in synthetic documentation provided to students. All students, divided into groups of three components, observed the

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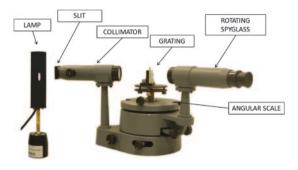


Fig. 1. – The optical goniometer. During the laboratory activity, students observed the discrete spectrum of a gas-discharge lamp, using it in order to measure the angles corresponding to the different wavelengths.

light pattern produced by the interaction of the light emitted from a gas-discharge lamp with a diffraction grating. The analysis was conducted at first at a qualitative level, observing the spectra corresponding to the various orders, then at a quantitative level by measuring the diffraction angle of every chromatic component and associating it with the corresponding wavelength and energy. Starting from the measure of an angle, students evaluate the corresponding wavelength using the formula $d \cdot \sin \theta = m \cdot \lambda$ and then they convert it into energy using the relation $E = h \cdot c/\lambda$, where h is Planck's constant and c is the speed of light.

Data were collected by means of both written questions using a tutorial and a posttest, and semi-structured and Rogersian interviews [36]. No pre-test was used. The tutorial, based on the one developed in [12], consisting of 9 open-ended questions, was submitted individually to the students asking them to argue their answers. The tutorial, conceived as an instrument of investigation rather than a support to the activity itself, was used after the experiment and students' answer were collected at the end of the whole activity. It made use of IBL strategies [31-33] and it was organized in stimulus-questions and in-context step-by-step analysis of interpretative aspects. The focus was set on the relationships between spectral lines energies and energy levels in the special case of the hydrogen atom, on the concept according to which the highest energy level in the atom is zero, on the fact that energy levels become closer together as the energy increases and on the relationship between the smallest and largest possible energies of the emitted light which correspond, respectively, to the smallest and greatest possible energy differences among levels, in order to collect students' reasonings. Interviews concerning the issues addressed in the tutorial were carried out during the laboratory activity. The post-test, delayed about 2 months, has been submitted individually to N = 45 students in the context of the final exam of the course. The post-test recalls the issues addressed in the tutorial, using 7 different open-ended key questions: it probes the students ability to associate any given spectral line with the transition between two specific energy levels and to sketch a qualitative energy level diagram from a given discrete spectrum.

The data collected were analyzed by qualitative methods [37,38] with operative definition of the different categories, identified *a priori* from the research literature and *a posteriori* form the specific sample's outcomes, in order to identify the number of non-mutually exclusive aspects present in the argumentation in every answer, the various types of aspects noticed and the conceptual referents underlying the interpretative models. The graphical representations used by students in order to explain their argumentations were analyzed and correlated with written answers.

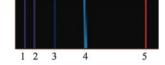


Fig. 2. - Balmer series: the optical emission spectrum of atomic hydrogen.

4. – Data analysis and discussion

4.1. Tutorial. – Here we report the analysis of the answers to the four most significant questions posed in the tutorial (numbered 3, 4, 5, 8). To question 3 (what is the shape of every line caused from?) half of the sample (26/56) answers that the shape of every line is due to the shape of the slit, while a significant fraction (22/56) states that the shape of the lines resembles the shape of the incisions on the grating. A little minority (5/56) argue that lines must be narrow in order to represent different specific energies.

Question 4 is particularly significant in order to analyze the different perspectives under which students interpret a discrete spectrum: the optical spectrum of hydrogen (Balmer series, fig. 2) is shown to students. They are asked to comment on a dialog between two students: the former states that red line in the spectrum corresponds to the higher energy level of the atom, since it has, among all, the greater wavelength; the latter states that the red line corresponds to the lower energy level (fundamental level) of the atom, since it has the lowest energy. Categories of students' answers are reported in table I.

From the analysis of the answers it emerges that one third of the sample (17/56)states, with high confidence, that every line in a spectrum is the outcome of a transition between two levels: these students disagree with both affirmations offered by the tutorial. One quarter of the sample (14/56), on the other hand, expresses, explicitly or implicitly, the idea that a single line corresponds to a single energy level. This denotes the tendency of associating a single emission to a single energy level. In particular, the red line, the one with the lowest energy, clearly corresponding to the smallest energy transition, was seen as equivalent to the fundamental level by half of the sample (27/56), probably due to the trivial interpretation of the formula linking energy and wavelength $(E = h \cdot c/\lambda)$ that could represent a formal ritual [39]. In fact this relation refers to the energy of the various emissions, and not to the energy of the levels, but only a little minority of the sample (3 students) states explicitly that, while 2 students state explicitly that the relation refers both to spectral lines and/or levels. A minority of the sample (20/56) disagrees with the affirmation that the red line corresponds to the fundamental level, arguing that it corresponds to the smallest energy transition. From the analysis of the students' answers different outcomes emerge: the problem of distinguishing the energies of the levels and the energies of the lines, the issue of giving sense to the two representations, as well as the need to discuss the formal relations in order to avoid them to become rituals that affect the interpretative reasonings.

In the following question (question 5) students are asked to compare the five energy values of the different emission lines with the values of the seven lowest energy levels for hydrogen in order to find a relationship between the two entities. On the basis of the relationship, they are asked to describe what happens to an atom when a photon is emitted. After doing that, students are asked to review their answers to the dialogue in the previous question. Despite this experience should help students recognize their

Statement	"An observed line corresponds to an energy level."	
Agree (A)/Disagree (D) with examples of argumentations	14/56 (A) "Spectral lines represent levels with increasing energy."; "Line 5 is the one with the highest frequency, thus it is not a fundamental level."	17/56 (D) "Every line corresponds to the energy difference between an energy level and level 2."; "Lines represent a jump between two levels and non a single level."
Statement	"Red line is the fundamental level."	
Agree (A)/Disagree (D) with examples of argumentations	27/56 (A) "Frequency is inversely proportional to λ , according to $E = h \cdot f = h \cdot c/\lambda$. So the red line has lower energy than the violet one, in other words it is closer to the nucleus. We can say that, among all, the red line is the fundamental level."	20/56 (D) "In the spectrum I cannot identify the fundamental level because the color I see represents an energy difference, thus a jump between levels."; "The atom in the fundamental level does not emit and the lines represent a ΔE ."
Statement	" $E = h \cdot c / \lambda$ refers to levels."	
Agree (A)/Disagree (D) with examples of argumentations	2/56 (A) "Relation between energy and frequency is $E = h \cdot f$, moreover, $c = \lambda \cdot f$, so frequency and wavelength are inversely proportional. Red correspond to a greater wavelength and thus to lower frequency and energy, so it corresponds to the fundamental level of the hydrogen atom."	$3/56$ (D) " $E = h \cdot f$ refers to the energy of the radiation, so the red line is the one with lower energy."; "The energy of a single photon is $E = h \cdot f$."

TABLE I. – Students' answers to the second question of the tutorial: "Does the red line correspond to the fundamental level because it has, among all, the lowest energy?".

tendency to make the common error of associating a single emission line with a single energy level and help them strengthen their understanding of the correct reasoning, half of the sample (28/56) simply describe the emission process and only 22 students analyze the given numerical values. Out of them, 14 students use the numerical values in order to argue their reasonings concerning the process, 5 students use the numerical values as a starting point to describe the emission process, and 3 students simply analyze the numerical values without metioning the emission process. Students who analyze the numerical values of the energy levels and of the emission lines adopt different approaches: 13 students describe only a particular set of energetic values, 9 of them focus the attention on the energy of the emission lines underlying the relationship between energy and wavelength leading to the conclusion that the fundamental level is the one with lower wavelength, while 4 of them focus their attention on the energetic values of the levels. 9 students compare the two sets of energies, but only 4 of them notice that the energy of an emission line can be evaluated as a difference between two energy levels, while 5 students consider the two sets as representative of the same quantity. Working through

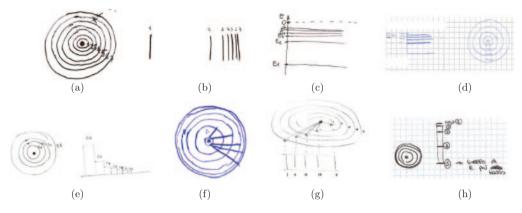


Fig. 3. – Tutorial: graphical representations of the energy levels.

this task, 9 students explicitly confirm their previous answer: 6 of them arguing that the red line in the spectrum represents the fundamental level, without recognizing that one of the students is incorrectly associating each emission line with a single atomic energy level; 3 of them arguing that a single line is the result of a specific transition. 3 students deny their previous answer stating that it is not true that the red line corresponds to the fundamental level, because negative values exist, it does not matter if they are referred to levels. It emerges that the majority of students starts from an idealized model rather than starting from the critical analysis of the data provided: they adapt the data to their description without using them as a starting point. 10 students state that the energy of the emitted radiation corresponds to a difference between energy levels, without correlations with the provided numerical values. The emission process is often described in a qualitative way in terms of the energetic jump of the electron (24/56) that gives back the absorbed energy (13/56), or in terms of the energetic variation of the atom (17/56).

In question 8, students are asked to sketch the energy levels for the hydrogen atom, observing their positions and relative distances. Data show that more than half of the students answering this question (29) use the classical representation that resembles the Bohr model, making use of orbits (fig. 3(a)). 17 students sketch levels distributed horizontally or vertically (figs. 3(b), (c)). 4 students make use of different representations at the same time, in particular 2 students couple an orbit-scheme with an energy level-scheme (fig. 3(d)), while 2 students couple an orbit-scheme with a sort of histogram (fig. 3(e)). Among students who use the Bohr representation, it emerges that 14 of them draw levels in number of 7, as the ones previously shown, only 1 student draws 6 levels (fig. 3(f)) and 2 students draw 5 levels (fig. 3(g)) in order to justify the five lines in the spectrum. 2 students quote the resulting spectrum (fig. 3(h)). Among students who use a level-scheme, the majority of them draws 7 levels, while the remaining draws an arbitrary number of levels, or a number with no link to the number of observed lines.

A spontaneous idea emerges: a single emission line is directly linked to an energy level of the emitting system. This representation, so common among university students, is a common feature of the first interpretations of atomic optical spectra in the history of physics, since scientists used to associate a single emission with a single harmonic oscillation in the atom [1].



Fig. 4. – Emission spectrum of atomic hydrogen shown to students in the post-test. Energy increases from left to right.

4.2. *Post-test*. – In the post-test students are shown a portion of the emission spectrum of atomic hydrogen in which 6 lines are present. The lines are grouped in three series, which is what is expected to see if only the four lowest energy levels are involved: the fundamental one and the first three exited levels (fig. 4).

Here we report the analysis of the answers to the first six questions of the post-test.

Students' answers to question 1, "How are the lines in the spectrum and the energy levels of the emitting system related?", fall into three main categories: one third (15/45) of the sample states that a line in the spectrum corresponds to a single energy level (examples of students' argumentations are "The relation between spectral lines and energy levels is expressed by Planck's formula: $E = h \cdot f = h \cdot c/\lambda$."; "Every line in the spectrum corresponds to a specific energy level of the considered system."); 10/45 students state that a single emission line corresponds to a difference in energy betwen two levels ("Lines correspond to a jump between an energy level and another one: when this happens, radiation is emitted."; "Electron in high energy levels is unstable and tends to return to the level with lower energy, so it emits a photon whose energy is equal to the energy difference between the two levels."), a minority of the sample (4/45) relates the number of series to the number of energy levels ("The first line represents the source, the second two lines represent the wavelengths of the first level, and the last three ones represent the wavelengths of the second level.").

In question 2, students are asked to identify the minimum number of energy levels required to produce the part of the spectrum shown, making a sketch of them. 8/45 students draw levels in number of 6, directly associating an emission line to an energy level, 6/45 students draw 7 levels associating a line to a level, adding the fundamental one, 5/45 students draw 3 levels, counting the number of series, 3/45 students draw 7 levels associating the number of series, 3/45 students draw 3 levels, counting the number of series, 3/45 students draw 3 levels with no justification and 2/45 students draw 4 levels in order to account correctly for the 6 emission lines observed (fig. 5). The majority of the sample make use of the "Bohr

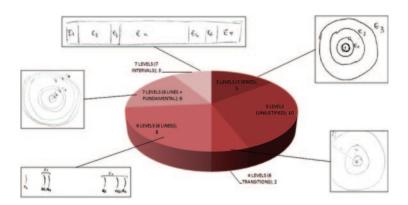


Fig. 5. – Post-test: graphical representations of the energy levels.

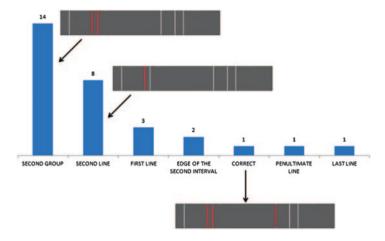


Fig. 6. – Post-test: lines involving energy level E_2 . Student's answers.

orbit representation" (25/45) rather than a "level representation" (13/45).

Post-test question 3 states: "The energy level E_2 (the first excited level) is involved in the formation of one, or more than one, line(s) in the spectrum. Show the line(s) involving level E_2 ." One third of the sample (14/45) identifies the second two lines starting from the left: this may be caused by the interpretation that a group of lines corresponds to a level, or by the interpretation that the involved level is considered only as the final level. 8/45 students identify the second line starting from the lower energy part of the spectrum, associating a single line with a single energy level. Various other answers are present, but hardly interpretable. A single student identifies correctly the three lines whose transitions involve level E_2 (fig. 6).

In question 4 students are asked how many new lines would be formed if the next higher energy level were taken into account. They are also asked to indicate the position(s) of the added line(s) in the spectrum. The student's answers to this question fall into three main categories (fig. 7): 12/45 draw a single higher energy line at in the right portion of the spectrum (fig. 7(a)); 5/45 students expect 4 lines at higher energy (fig. 7(b)) and 1/45 student gives the correct answer in terms of transitions, though he does not represent the lines in the spectrum.

Question 5 states: "For atomic hydrogen, the energies of the fundamental level E_1 and E_3 are respectively -13.61 eV and -1.51 eV. Which line(s) is (are) possible to predict in the spectrum? Evaluate its/their energy/energies." Instead of evaluating the difference

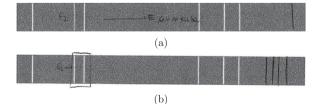


Fig. 7. – Post-test: position(s) of the line(s) formed taking into account a higher energy level. Student's answers.

between the two given energy levels, 11/45 students associate directly a wavelength to the given two energies, according to the ritual $E = h \cdot c/\lambda$ while 12/45 students perform unclear calculations involving differences between couples of values, highlighting the lack of conceptul understanding.

The tendency to associate a single emission line to a single energy level is more prominent in the post-test than in the tutorial, due to the fact that no suggestion concerning energy levels values was provided to students: they could only rely on the observed spectrum.

In question 6 students are asked what they expect to observe if the grating is removed. The majority of the sample (32/45), focusing on the descriptive plan, states that the lines will no longer be visible, due to the fact that the grating's function is to separate the different wavelength. 6/45 students say that lines are always visible, in fact the grating's role is to make a discrete spectrum more definite, while 5/45 students, focusing on the intrpretative plan, state that diffraction will no longer occur.

5. – Conclusions

A research-based intervention module on optical spectroscopy for freshmen in biotechnology was designed in order to gain competence on students' learning processes using a tutorial in a laboratorial context, and a post-test.

The specific roles of the diffraction grating and the slit (RQ1) require a particular additional discussion for half of the students who look at the diffraction grating as responsible for the shape of the spectral lines. More than 10% of students expects to observe spectral lines also when removing the grating. These evidence seem to be correlated to the great conceptual change involved in the explanation of the existing difference between a diffraction pattern and a discrete spectrum. Qualitative plan prevails in students' description of the emission of light from an atom: students quote energy changes but when they are provided energy values for levels and lines, they do not correlate the two sets by means of the simple relationship existing between them. It seems that the formal relationship between energy levels and spectral lines have to be specifically addressed (RQ2). Concerning the reasonings and representations used in order to describe the relationship between the two different referents (RQ3) it emerges that the term "energy level" is misused: spectral lines of higher energy are quoted as greater "energy levels". Explicitly, sometimes single lines are related to single levels. This result offers us students' way of thinking when we correlate it with other outcomes already outlined in literature [11-13] concerning students' perspective in which the fundamental level has zero energy and it is involved in every transition. Despite an explicit qualitative comparison between lines and levels energies was offered to students in the tutorial, the problem of the conceptual link between the two referents appears in the post-test as a lack of functional understanding of the topic.

Findings of the study here presented suggest the need of devoting more time and attention to the phenomenological exploration and discussion of hypothesis at the base of the experimental work in order to gain a deeper conceptual understanding of every component of the setup. The surprising lack of spontaneous use of simple mathematical operations linked to the processes under analysis, also when all the elements are provided to students, suggests working in gaining ownership with modalities in which it is possible to obtain information from the relationship between spectral lines and energy levels. This is particularly important in the conceptual distinction between continuous and discrete spectra. * * *

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