HOW TO TEACH ATOMIC STRUCTURE USING COMPUTER SIMULATIONS OF FUNDAMENTAL EXPERIMENTS AND HEURISTIC DIAGRAMS FOR HISTORICAL CONTEXT

José A. Chamizo

Facultad de Química, UNAM, México D.F. (México)

ABSTRACT

Information and Communication Technologies (ICTs) have so far had little impact in the Historical Teaching of Atomic and Molecular Structure with the exception of graphs of orbitals, electron densities and contours. The PhET project (Physics Education Technology) was designed to help students grasp fundamental scientific principles. To date, over 130 simulations in several sciences have been used more than 75 million times a year by students worldwide. Some of the designed computer simulations have been devoted to atomic and molecular structure from historical experiments, but important as this material is the failure to address historical context and provide historical references has made this approach so far weak.

Heuristic diagrams (HD) are graphic organizers. Its main feature is the possibility it entails for relating conceptual frameworks, research questions and research outcomes. HD can be used as a tool to develop research because it helps identifying all the elements of an specific investigation.

The PhET computer simulations and the HD were used with teachers in a General Chemistry Course in a Master degree in the Universidad Nacional Autónoma de México (UNAM). PhET computer simulations of fundamental experiments in atomic and molecular structure were performed (for example Photoelectric effect, Davisson-Germer or Stern-Gerlach experiments). Every teacher produced two HD related with every PhET computer simulation. The results of this process indicate a greater and deeper understanding of the experiments by teachers. Besides, the possibility to contextualize these experiments historically through the HD, allows them to recognize their value not only in the history of science but also as an educational resource.

Keywords: Heuristic Diagrams, Atomic structure, computer simulations, history of science.

1 INTRODUCTION

After the fourth chemical revolution (1945-1965) [1], the hegemony of physical chemistry would provide a basis of understanding for students' introduction to the chemical sciences mainly through the quantum chemistry basis of atomic structure and the chemical bond. The General Chemistry courses turned towards a theoretical character, losing the phenomenological approach that it had in the preceding years. Without a deep recognition of its historical and philosophical roots, many people were led by this approach to believe that the contents of science textbooks were, in fact, science. However this is not necessarily true. The written materials employed in science education are descriptions of past science explorations [2]…and not the best ones! For example, some scholars [3] examined numerous textbooks for the History and Philosophy of Science (HPS) content in their approach to teaching atomic structure, and they found that an adequate and accurate reflection of the historical development is rarely presented. About that has been showed [4] that the concepts and processes of quantum chemistry are abstract and complex so students have to resort to rote learning of definitions, formulas, and process. This is educationally significant because philosophers of science and science education researchers have argued that quantum mechanics is particularly difficult to understand, due to the intrinsic obscurity of the topic and the controversial nature of its different interpretations [5].

Experiments related to the history of atomic and molecular structure are rare. However, there are some examples, ranging from the electrochemical decomposition of water to spin through the Stern-Gerlach experiment [5]. For this reason Information and Communication Technologies (ICTs) appears to be a good didactical alternative to teach this subject. However the challenge about information is not only quantitative but also qualitative. Generally speaking currently we process more information in 24 hours than the average person would process in a lifetime 500 years ago, when the fundamental structure of today's university was solidly established [6]. In this context the aim of education cannot be only informing. The idea will be to help students to reason through scientific thinking rather than to regurgitate the conclusions of science. Generally speaking, scientific content is taught, but Schwab's [7] interpretation of science teaching as a dogma or as "*a rhetoric of conclusions*" remains. It means that if scientific competence is not worked out, we cannot say that scientists are being trained. On this subject there are different positions, but it is possible to recognize that scientific activities, particularly experimental ones, requires more reflection and less memory [8]. One way to do that it is to scaffold teachers in open-inquiry teaching [9].

The PhET project (Physics Education Technology) developed at the University of Colorado are designed to help students grasp fundamental scientific principles. To date over 130 simulations in physics, biology, chemistry, earth science and math — translated into 78 languages — have been used more than 75 million times a year by students worldwide (http://phet.colorado.edu). Some of the designed computer simulations have been devoted to atomic and molecular structure from historical experiments. PhET conducts research on both the design and use of interactive simulations [10][11], but important as this material is, the failure to address historical context and provide historical references has made this approach not as good as could be.

2 HEURISTIC DIAGRAMS

Learning in the real world is a product of problem solving. Students who are actively engaged in the educational process make substantial connections with course content. These connections promote a deep level of processing [12]. For example, requiring students to ask questions, generate ideas and provide explanations to support those ideas promotes learning [13]. This is a new teaching culture where the capacity to form questions is more valued than that of giving unasked, or simple answers. In accordance with the French philosopher G. Bachelard [14]:

And say what you will, in the scientific life problems do not arise by themselves. It is this sense of the problem that indicates the true scientific spirit. To a scientific mind all knowledge is the answer to a question. If there was no question, there can be no scientific knowledge. Nothing is spontaneous. Nothing is given. Everything is built.

So is reached the issue that matter most to us. Of that it is for students get an open question, a

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question that defines a specific problem in a particular historical moment related with atomic structure' experiments.

Heuristic diagrams (HD) are graphic organizers and an improvement of Gowin's Vee [15]. Graphic organizers represent thinking processes; they can be regarded as a 'cartography of cognition' that makes learning visible [16][17]. Gowin recognized the initial difficulty of students in producing Vees, particularly the time required becoming competent, but he also recognized its value. Its main feature is the possibility it entails for relating conceptual frameworks, research questions and research outcomes [18]. The heuristic Vee is composed of five parts: events or phenomena to be researched, the research question, a methodological part, a conceptual part, and the answer to the research question. One of the main features of heuristic Vee is that it explicitly relates the conceptual-theoretical aspects of a research question with the practical aspects allowing for this constant interplay. Despite its virtues, one of the greatest difficulties in the use of Gowin's Vee is due to the ambiguity of its left side, one that regards concepts.

Heuristic Diagrams incorporates Stephen Toulmin philosophical approach [19]. Toulmin's work [20] recognizes the complexity inherent to concepts through its historical-social interactions. Just as Vee diagrams, Heuristic Diagrams can be used as a tool to develop research: in teaching history [21]; or in laboratory assessment [22]; or as a tool to assess teacher's research [23]; or to facilitate the acquisition of argumentative competence [24]. All these because it helps identifying all the elements of the investigation, mainly under the Problem Based Learning (PBL) approach [25]. About this "dialectical circle", in which one starts with a question, and both, the concepts and the methodologies become "visible", Trowbridge and Wandersee said [16, p.115]:

You focus on the research (or focus) question and decide what is that you want to study elaborating the methodological side. Next, develop the theoretical side and you will be able to see how theory (concepts) affects and modify practice. Once the research is done you will be able to see even more how practice affects theory and vice versa.

One of the main improvements of HD is that it brings more clarity to the conceptual part of the heuristic Vee. The HD recognizes that each concept requires three different aspects for its complete understanding: applications, language and representation techniques, it means models [26]. Reflection on these different aspects allows for a more thorough comprehension of the conceptual elements that are relevant to any given investigation. The events or facts that induce the question must be recognized through literature references at a specific historical moment and the answer to the question must be explicit. The right column allows students self-assessment in accordance with a specific rubric (Appendix).

To begin working with this graphic organizer it is necessary to construct a question, as proposed by Bachelard, from facts. This is not an easy task and students should learn how to do it. Therefore after reviewing several taxonomies [27] we recognize two extreme types of questions, closed and open that can be characterized as follows: Closed (request information from one source and the answer is short and in one place); Open (evidence and information requests from two or more sources, the answer is broad, refers to analysis, appeals for the organization of ideas, concepts and facts and establish relationships among them). Hence asking requires, from the person doing it, mobilizing knowledge and skills, and recognizing the depth of his own knowledge. Questions should be well formulated (precise and clear), unambiguous,

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contextualized (in time and space) and feasible (that can be answered by the person who asks).

3 DESCRIPTION OF AN INTERVENTION USING HEURISTIC DIAGRAMS

The PhET computer simulations and the HD were used with teachers in a 16 week Intermediate General Chemistry Course in a Master degree in the Universidad Nacional Autónoma de México (UNAM). Besides the use of other educational materials (“Modeling the Black Box” [28]) and “The Shell Model of Atoms to Explain Ionization Energies” [29]) four of more than ten PhET computer simulations of fundamental experiments in atomic and molecular structure were performed (Neon lights and other discharge lamps, Photoelectric effect, Davisson-Germer and Stern-Gerlach experiments). The Appendix of this article indicates the instructions to fill in the HD, taking into account that it should not occupy more than one page. Every teacher produced two HD (one per week) related with every PhET computer simulation. The rubric for self-assessment was constructed through a discussion with teachers-students with the aim of not only assessing the HD but also to serve as a guide for learning. It means that two sessions were devoted to each simulation. Teachers used the “Teaching Resources” than came with each simulation in order to understand more deeply the content and the experimental details. None of them are related with the historical facts behind the experiments. All diagrams were collected during the course and students were interviewed at the end of the semester to find out how useful they thought heuristic diagrams were.

4 RESULTS

Along the intervention students refine the questions they are asking; through research and in-class discussion, teachers-students modify their initial questions to encompass their interests and consider methodological (improve the use and understanding of the simulation) and conceptual (historical) issues. For example in figures 1 and 2 this particular teacher goes from two to one question and from close to open question. As was recognized [30]: *Teaching students categories of question types can make them aware that different kinds of questions elicit different thinking processes that help build answers in different ways that can lead to insight.* The reiterative use of HD helps teachers-students in developing such skill. Progression in questions coincide with previously expressed views [31] in the sense: *There is ample empirical evidence that students can be trained to ask good questions and that such training leads to significant gains in learning and literacy.*

These progressions in HD’s help asking, making learning visible [9]. For example as can be seen in Fig. 1 and 2, Facts, Data Collection, Conclusion, Answer and Self-assessment changed. One of the teachers indicated:

You need to consider the filling of the heuristic diagram is a cyclical process. The facts should help raise the question correctly, language is the necessary terms that should allow us to answer, model must explain the answer. The result is the answer or solution to the question considering the conceptual and methodological part. Finally, one should read the finished heuristic diagram to see if it meets all.

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Figure 1. First Heuristic Diagram

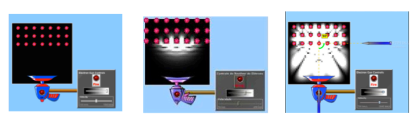
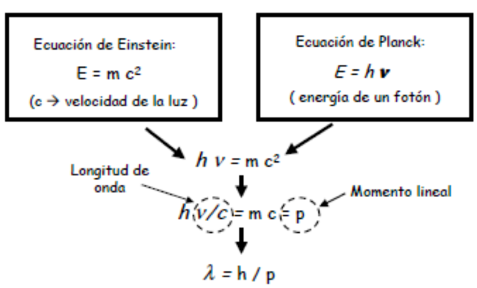
<table>
<tr><td colspan="2">HEURISTIC DIAGRAM ABOUT: DAVISSON-GERMER’ EXPERIMENT</td><td>Pts</td></tr>
<tr><td colspan="2">FACTS
1. De Broglie raises the possibility that in the case of a particle such as an electron, h be related to some kind of wave behavior.
2. In 1925, Einstein observed that a beam of molecules should show small but measurable effects of diffraction.
3. Diffraction occurs when the wavelength is equal to or greater than the characteristic size of the obstacle.
4. The crystals form "slots" of small size where waves of short wavelength are diffracted.</td><td></td></tr>
<tr><td colspan="2">QUESTION
Do particles have dual nature of wave and corpuscle?
How would you show you that an electron can behave like a wave?</td><td></td></tr>
<tr><td>CONCEPTS</td><td>METHODOLOGY</td><td>0</td></tr>
<tr><td>Applications
X ray diffraction</td><td>Data
Simulation of Davisson-Germer’ experiment</td><td></td></tr>
<tr><td>Language
whole number n
wave length λ
frequency ν
Planck constant
Speed of light c</td><td>Data processing

Bragg diffraction law dsenθ = nλ</td><td></td></tr>
<tr><td>Model

</td><td>Conclusion
Electrons, and by extension all particles of small mass, exhibit wave’s characteristics</td><td></td></tr>
<tr><td colspan="2">ANSWER or RESULT
De Broglie proposed that the relation λ = h / p was also valid for a particle of matter and not just for a photon.
The electrons experience a diffraction electron wavelength given by λ = h / p
Davisson-Germer’ experimental results confirmed de Broglie assumption.</td><td></td></tr>
<tr><td colspan="2">REFERENCES
Facts: http://books.google.com/books?id=1_AuxY6QjbsC&pg=PA154
Concepts: http://www.geothesis.com/index.php?option=com_content&task=view
Methodology: http://phet.colorado.edu/en/simulation/davisson-germer</td><td></td></tr>
<tr><td colspan="2">Self assessment</td><td></td></tr>
</table>

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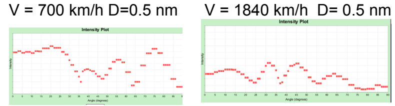
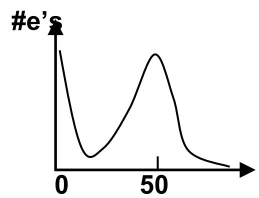
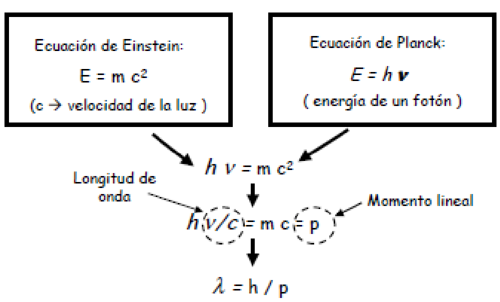
Figure 2. Second Heuristic Diagram

<table>
<tr><td colspan="2">HEURISTIC DIAGRAM ABOUT: DAVISSON-GERMER' EXPERIMENT</td><td>Pts</td></tr>
<tr><td colspan="2">FACTS 1. Diffraction occurs when the wavelength is equal to or greater than the characteristic size of the obstacle. 2. The crystals form "slots" of small size where waves of short wavelength are diffracted.</td><td>2</td></tr>
<tr><td colspan="2">QUESTION
Why, when an electron beam is fired into a network of nickel atoms, the electrons are detected only at certain angles?</td><td>3</td></tr>
<tr><td>CONCEPTS</td><td>METHODOLOGY</td><td>0</td></tr>
<tr><td>Applications
Electron microscopy</td><td>Data
Simulation of Davisson-Germer' experiment</td><td>2</td></tr>
<tr><td>Language

Wave length (λ)
Frequency (ν)
Planck constant (h)
Speed of light (c)</td><td>Data processing
V = 700 km/h D=0.5 nm   V = 1840 km/h D= 0.5 nm


</td><td>2</td></tr>
<tr><td>Model

</td><td>Conclusion
Electrons diffracted from a crystal lattice of nickel atoms especially at certain angles due to wave interference. For example it can be seen that at a speed of 700 km/s the wavelength is less than 1840 km/s maintaining constant diameter D = 0.5 nm. At 50 degrees diffraction is higher, hence more electrons are diffracted.</td><td>3</td></tr>
<tr><td colspan="2">ANSWER
Because electrons are diffracted. Their wavelength is given by the equation λ = h / p. At a certain angle (50) more electrons are diffracted.</td><td>2</td></tr>
<tr><td colspan="2">REFERENCES
Facts: http://books.google.com/books?id=1_AuxY6QjbsC&pg=PA154
Concepts: http://www.geothesis.com/index.php?option=com_content&
Methodology: http://phet.colorado.edu/en/simulation/davisson-germer</td><td>3</td></tr>
<tr><td colspan="2">Self assessment (addition of all points)</td><td>17/20</td></tr>
</table>

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So she had to read the original article, which despite its conceptual complexity, the apparatus used (than in PhET simulation is reproduced in simplified form) and the most important result was recognized [32 p. 707]:

Because of these similarities between the scattering of electrons by the crystal and the scattering of waves by three- and two dimensional gratings a description of the occurrence and behavior of the electron diffraction beams in terms of the scattering of an equivalent wave radiation by the atoms of the crystal, and its subsequent interference, is not only possible, but most simple and natural. This involves that association of a wave-length with the incident electron beam, and this wave-length turns out to be in acceptable agreement with the value h/mv of the undulatory mechanics… That evidence of the wave nature of particle mechanics would be found…after the appearance of L. de Broglie's original paper on wave mechanics.

On average teachers require one hour performing each simulation and two hours filling its heuristic diagram. It means that at least they employ six hours by themselves and at least two more in a sharing discussion about each simulation.

Final comments of two teachers about this intervention were:

PhET simulations allowed obtaining experimental results from modifying variables and significantly deepening the conceptual understanding of the subject.

The great advantage of a heuristic diagram is the simplicity of having everything on one sheet where the conceptual and methodological parts are included. So the student must achieve to bring together those two parts, and not see them isolated, as often it happens in experimental reports.

5 CONCLUSIONS

The results of this process indicate a greater and deeper understanding of the experiments by teachers. Besides, the possibility to contextualize these experiments historically through the Heuristic Diagrams, allows them to recognize their value not only in the history of science but also as an educational resource.

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APPENDIX. Instructions for completing a heuristic diagram and scoring rubric

TITLE: (Refers to the subject of research)		Pts
FACTS: (This refers to information obtained and / or observations about something happening in the world that leads us to ask a question. Preferably should identify several of them)		
QUESTION: (Statement of an inquiry focusing on the facts. We must make sure that there is only one question)		
CONCEPTS	**METHODOLOGY**	0
Applications (Refers to applications for the issue under investigation)	**Data collection** (This refers to what we do to obtain the relevant information to answer the question. It should be pointed and detailed)	
Language (Refers to the terms we need to know to answer the questions)	**Data processing** (Refers to data management and results in tables, charts, diagrams etc. which summarize the data obtained)	
Models (This refers to the model used to give the answer to the question. It may be scientific, economic, social, etc. For example Lewis' atomic model, or Arrhenius' acid-base model, or market model, constructivist learning model, etc..)	**Conclusion** (This refers only to that obtained from the processed data)	
ANSWER or RESULT: (Refers to the explanation that answers the question by bringing together the concepts and methodology's conclusion) or in case that there is no answer the result of the research		
REFERENCES: (This refers to books, magazine articles, websites, etc., consulted and used in every part of the investigation)		
Self assessment (addition of all points) (You need to score all the points collected and compared against possible points)		

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Points	Characteristics
	FACTS
0	No facts
1	Some facts are recognized
2	Facts are recognized and some concepts
3	Facts and concepts are recognized and also some methodological aspects
	QUESTION
0	No question
1	There is a question related (supported) with facts
2	There is a question related (supported) with facts that includes concepts
3	There is a question related (supported) with facts that includes concepts and suggests some methodological aspects
	METHODOLOGY
0	No methodology
1	There is a procedure that allows data collection
2	Data processing (tables, graphics)
3	A conclusion has obtained through data processing
	CONCEPTS
0	No concepts
1	Applications are identified
2	Applications and language are identified
3	Applications and language are identified and also models capable to explain the question
	ANSWER
0	No answer
1	Answer is quite similar to methodology's conclusion
2	Answer besides methodology's conclusion includes facts
3	Answer besides methodology's conclusion includes facts and concepts (models particularly)
	RESULT
0	No result
1	Errors are identified
2	Errors are identified and explained
3	Errors are identified and explained and a reasonable alternative solution is proposed
	REFERENCES
0	No references
1	There are references related only to facts, concepts or methodology
2	There are references related to facts, and concepts or methodology
3	There are references related to facts, concepts and methodology

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