Strasbourg Students Physical Letters

Teaching Quantum Mechanics to Seconde Interns

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As of the academic year 2023-2024, Seconde (10th grade) students are required to complete an internship in a private or public organization. Laboratories and research institutions are solicited to host some of these interns, but it appears difficult to provide them with scientific knowledge affordable at their educational level. This paper summarizes efforts made at the Quantum Chemistry Laboratory of Strasbourg to teach the basics of Quantum Mechanics and Chemistry to two Seconde students that interned there. The scientific content of the internship included the shell model of the atom, Lewis' theory of the chemical bond, the postulates of Quantum Mechanics, the two-level system, and a discussion of various approaches to chemical bonds and reactions.

INTRODUCTION

In the French education system, the class of *Seconde* (corresponding to the 10th grade) is the first year of the *Lycée* (roughly corresponding to High school), immediately followed by the classes of *Première* (11th grade) and *Terminale* (12th grade). Since 2024, Seconde students are required to complete a two-week internship in a chosen organization or institution. The Quantum Chemistry Laboratory of Strasbourg hosted two of these interns at the end of academic year 2023-2024.

We are faced with two major difficulties when introducing Quantum Mechanics to Seconde students. On the one hand, their lack of mathematical knowledge forces us to work with hardly more than vectors (in two or three dimensions) and functions (from $\mathbb{R}$ to $\mathbb{R}$). Indeed, derivatives, integrals, matrices and complex numbers are only taught in Première and Terminale. On the other hand, their lack of knowledge in physics prevents us from using Newtonian Physics as a basis onto which Quantum Mechanics can be elaborated, since Newton's Laws of motion are not tackled before Terminale. This is of course a huge drawback, as the usual way to introduce Quantum Mechanics consists in quantizing Classical Hamiltonians, and in using wavefunctions that obey a complex differential equation (the Schrödinger Equation) [1].

It would have been possible to discuss some simple experiments only (like Young's double-slit interferometer), and avoid diving into theoretical details. This is besides the usual path taken by popular science, but such an approach cannot lead us very far, notably when we want to explain the quantum nature of chemical phenomena [2], and it seemed more interesting to take advantage of the full-time two-week presence of the interns to provide them with a true introduction to quantum theory.

The structure of this paper follows the steps of the internship. In the first instance, as recalled in Section I, we presented the atom's shell model and Lewis' chemical bond theory [3], which can be applied without any reference to the principles of Quantum Mechanics, but where quantum effects can be detected. Comparison with experiment led us to look for a more advanced theory of quantum phenomena.

Section II begins with the introduction of general n-dimensional vectors and matrices, and shows how such simple mathematical tools (quite accessible to Seconde students) can be used to present the postulates of Quantum Mechanics, with the notable exception of the Schrödinger Equation (dynamics will not be tackled here). As an illustration, we diagonalized the two-level system Hamiltonian and, interpreting it as two spatially separated hydrogen atoms, used it as a model to justify the formation of bonding orbitals between the two atoms, and thus the formation of the H_2 molecule.

Quite surprisingly, this already busy agenda was completed during the first week of the internship. We decided to further the lesson on the chemical bond by discussing covalent bond formation from different points of view that all reveal quantum effects (see Section III).

The interns were also involved in other activities (programming courses, lab visits, scientific seminars, etc.), but we will not discuss them here, as it goes beyond the scope of this paper, namely the teaching of Quantum Physics.

This paper will not address the physics itself, as the reader is assumed to be familiar with Quantum Mechanics, but rather the strategies that can be enforced to teach this physics to Seconde students.

I. THE QUANTUM NATURE OF ATOMS AND MOLECULES

Our first task was to put Quantum Mechanics in the zoology of physical theories, to make the interns understand what Quantum Mechanics *is* and what it is not. For this purpose, we explained the genealogy of physical theories as represented in Fig. 1, starting with the XIXth century (Thermodynamics, Classical Mechanics and Electromagnetism), immediately followed by the 1905 *annus mirabilis* (Special Relativity and Quantum Mechanics), which led to further developments in the

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XXth century (Quantum Field Theory and General Relativity). In the light of this historical explanation, Quantum Mechanics is correctly delineated as the theory of small objects with low speed.

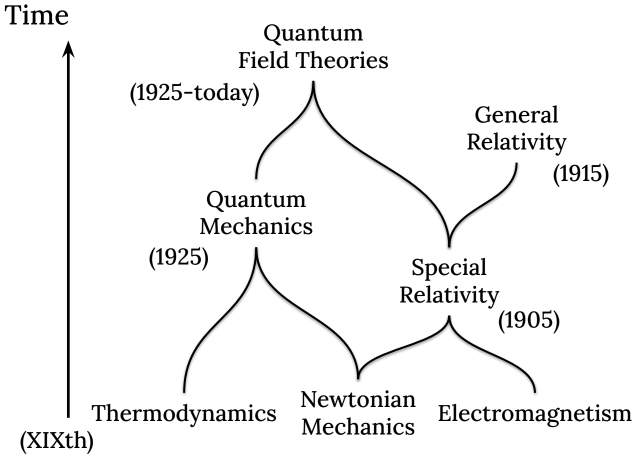


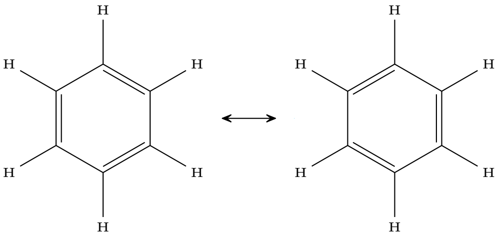
FIG. 1: Simplified genealogy of modern physical theories (superstring theories can be added at the top as they are a prominent subject in popular science).

Then, we began our journey through quantum theory by explaining a few historical models of the atom, culminating in the shell model. We introduced the four atomic quantum numbers, Pauli's exclusion principle, the aufbau rule and Hund's rule. With this, valence calculations are made possible, and Lewis' covalent bond theory can be easily tackled, together with the concepts of single electrons, (non-)bonding pairs and double bonds. It is interesting to emphasize the definition of a covalent bond as a *sharing* of two electrons. Indeed, Classical Mechanics cannot make sense of this, and the quantum concept of *delocalization* is needed for the first time.

This exposition must be concluded by presenting some deficiencies of the atomic shell model and Lewis' subsequent theory. First, a number of elements violate the aufbau rule (*e.g.* chromium and other elements from the 4th period and above). Indeed, a general atomic state should be seen as a quantum superposition of configurations, and not as a single configuration.

Secondly, there are inconsistencies in Lewis' theory, as carbon (for instance) should have one non-bonding pair (the 2s electrons) and two single electrons (the 2p ones). Instead, all valence shell electrons are considered equivalent when applying Lewis' theory, and carbon has four single electrons, which is confirmed by experiments. Chemists account for this change of orbitals with hybridisation theory, betraying changes in the shell structure when the atom interacts with electrons from other atoms.

Finally, a famous limitation of Lewis' theory is *mesomerism*, when several Lewis structures must be used to describe a molecule completely. A typical example is benzene, whose possible Lewis structures show an alternation of simple and double bonds:



However, experiments reveal that all bonds are equivalent (they have the same length and the same strength). This shows that electrons can be delocalized between more than two atoms, questioning the very concept of covalent bond as it is defined by Lewis' theory.

II. INTRODUCTION TO QUANTUM MECHANICS

This is where difficulties begin. Section I was intended to be a simple introduction to some quantum effects, leading us to conclude that a better theory of the quantum world is needed to obtain a correct depiction of atoms and molecules. However, discussing wavefunctions seems impossible, as we would need to introduce derivatives for some of the operators, integrals for expectation values, or complex numbers for the Schrödinger equation. Fortunately, there is quite a profusion of different formulations of Quantum Mechanics, and it appeared to us that the matrix formulation could prove simple to teach as well as a convenient way to introduce most concepts of Quantum Chemistry.

A. Vectors and matrices

And so we defined n-dimensional vectors and square matrices as collections of (real) numbers ordered in tables:

$$v = \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix} \quad ; \quad M = \begin{bmatrix} M_{11} & \cdots & M_{1n} \\ \vdots & \ddots & \vdots \\ M_{n1} & \cdots & M_{nn} \end{bmatrix} \tag{1}$$

Then, we explained how such objects can be added and multiplied, insisting on non-commutativity and on the interpretation of square matrices as functions associating a vector to another vector.

After a few exercises, we also discussed transposition and its properties (*e.g.* cyclic reordering), leading us to defining covectors as collections of numbers ordered in a line table:

$$\begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix}^T = \begin{bmatrix} v_1 & v_2 & \cdots & v_n \end{bmatrix} \tag{2}$$

Then, the inner product of vectors can be defined as:

$$u \cdot v = u^T v = u_1 v_1 + u_2 v_2 + \cdots + u_n v_n \tag{3}$$

From there, Dirac notation is introduced without difficulty: kets are vectors, bras are covectors, operators are square matrices and all products are matrix products (we did not use direct products in this internship, so expressions like $|\phi\rangle\langle\phi|$ were not discussed, although they could have been introduced symbolically from their effect on bras and kets).

B. The postulates of Quantum Mechanics

This is all the mathematical apparatus we need. The postulates of *stationary* Quantum Mechanics (*i.e.* excluding the Schrödinger Equation) can be successfully taught from this point. Throughout this presentation, it is very important to insist on the connection with experiment and measure. The postulates are *not* mathematical abstractions!

Postulate I. The state of a quantum system is completely characterized by a state vector. "Completely characterized" will be precised by the following postulates. Collinear vectors determine the same quantum state, hence the normalization, and the zero vector is not a quantum state.

Postulate II. Each physical observable is represented by a symmetric operator, in the sense that measurable quantities are precisely its eigenvalues. Of course, eigenvalues and eigenvectors need to be defined! Eigenvectors with different eigenvalues are orthogonal. A n-dimensional operator has exactly n orthogonal eigenvectors. $|1\mathrm{s}\rangle$, $|2\mathrm{s}\rangle$, etc. are energy eigenstates of the hydrogen atom (this remark is important, as it makes the connection with Section I).

Postulate III is Born's rule. This postulate allows us to justify the normalization condition and to interpret eigenstates as states in which the observable's value is known with certainty. The concept of *superposition* is introduced in opposition to eigenstates. (A small exercise is relevant at this point to apply the first three postulates to an example quantum state.)

Postulate IV describes spontaneous collapse. This is one of the great strangenesses of Quantum Mechanics: why is superposition destroyed by observation?

Postulate V would be the Schrödinger Equation. We can explain that finding the energy eigenstates is the central problem of Quantum Mechanics, since solving it also yields the time evolution of quantum states.

At this point, a "general quantum mechanical method" should be laid out for the students. The main idea of such a method is to decompose the reasoning on a quantum system in (more or less) the following steps:

1. A system is described by its Hamiltonian, so we need to write it, but learning how it can be constructed is out of the internship's scope, so the interns will always be given the Hamiltonian.

2. We compute the eigenenergies and associated eigenvectors. Unfortunately, there is no general method to perform this computation. An example will be given in Section II C.

3. A ket $|\psi\rangle$ be given, we can decompose it as a superposition of energy eigenvectors. The coefficients are obtained through inner products and their square is the probability of measuring the associated energy.

4. For a different observable, the same ket admits a different decomposition as a superposition of eigenvectors. The coefficients are still obtained through inner products and their square is now the probability of measuring the associated observable eigenvalue.

C. The two-level system

These postulates must be illustrated by working on a simple example. With the sole mathematical tools from Section II A, it is possible to solve the eigenvalue problem of a two-level system.

The two-level system is explained as consisting of two sites that each contain an atom. An electron is allowed to travel between them, so the system can be either in state $|0\rangle$ (if the electron is in site 0 located at $x = -1$) or in state $|1\rangle$ (if the electron is in site 1 located at $x = +1$). In this situation, $|0\rangle$ and $|1\rangle$ are position eigenstates. The interns may be asked to check that the position operator is of the form:

$$\hat{X} = \begin{bmatrix} -1 & 0 \\ 0 & +1 \end{bmatrix} \tag{4}$$

This tests their understanding of the eigenvalue problem (postulate II).

Then, two cases are successively examined. First, we assume that the two sites are non interacting, and we fill them with, for instance, a hydrogen atom of energy $\varepsilon_0 = -13.6\,\mathrm{eV}$ and a lithium atom of energy $\varepsilon_1 = -122\,\mathrm{eV}$. Analogously, the interns can be asked to justify that the Hamiltonian is of the form:

$$\hat{H} = \begin{bmatrix} \varepsilon_0 & 0 \\ 0 & \varepsilon_1 \end{bmatrix} \tag{5}$$

They must not only follow the same reasoning as for $\hat{X}$, but also explain that, in this case, $|0\rangle$ and $|1\rangle$ are also energy eigenstates.

As a second case, we can add an interaction between the sites. For simplicity, we suppose both sites to be occupied by a hydrogen atom of energy $\varepsilon = -13.6\,\mathrm{eV}$, interacting through a coupling $-J$, yielding a Hamiltonian:

$$\hat{H} = \begin{bmatrix} \varepsilon & -J \\ -J & \varepsilon \end{bmatrix} \tag{6}$$

the interns' attention may be drawn to the appearance of off-diagonal terms to represent the interaction.

Because we are working in 2D, the eigenvalue equation consists of two real equations, which can be interpreted as two geometrical straight lines. Now, two situations are possible: either these lines cross in a single point, or they are parallel. The system is easy to solve in the first situation, showing that the lines cross at the origin. However, we have already said that the zero vector is not a quantum state, indicating that this situation is impossible, and thus the lines are parallel. Parallelism can be mathematically enforced by equating the lines' slopes. By the miracle of linear algebra, this equation is the characteristic equation of $\hat{H}$, and it can be solved by the known identity:

$$0 = (\varepsilon - E)^2 - J^2 = (\varepsilon - E - J)(\varepsilon - E + J) \tag{7}$$

The eigenenergies are found without introducing the slightest notion of diagonalization theory. The eigenvalue equation becomes a simple linear equation, and together with the normalization condition, the eigenvectors can be easily retrieved.

Two things in this result can be discussed. First, one of the eigenenergies is lower than ε, leading us to conclude that it is interesting for two interacting hydrogen atoms to form a H_2 molecule. The essential argument here is energy minimization, a fundamental physical principle that should be addressed with the students. Secondly, the atomic orbitals (OAs) introduced in Section I mix to form *molecular orbitals* (MOs) depicted in Fig. 2, illustrating the delocalization of the electrons predicted by Lewis' theory (ask the interns to compute the probability of finding the electron on either site).

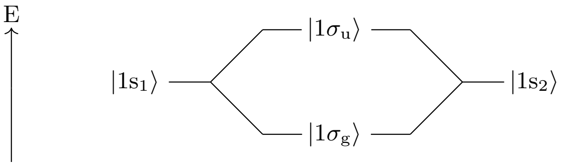


FIG. 2: H_2 molecular orbital diagram. The OMs are formed from the hydrogen 1s AOs.

III. CHEMICAL BONDS AND CHEMICAL REACTIONS

The discussion of Section II C can be generalized to an energy-based explanation of chemical bonds. Interacting AOs combine to form MOs, some of which are lower in energy (bonding orbitals) and some of which are higher (anti-bonding orbitals). This explains the duet and octet rules, along with bond order (explained also by the presence of non-bonding orbitals). These concepts are closely connected to the ones of bonding and non-bonding pairs in Lewis' structures. Besides, the importance of electron *pairs* is justified by spin and Pauli's exclusion principle.

From a spatial point of view, the formation of MOs induces the delocalization of the electrons over the whole bond. This can help introduce the notion of overlapping AOs forming covalent bonds. σ and π bonds can be discussed, with appropriate images showing the electron density distribution in each case. Double bonds are the combination of a σ and a π bond, which has several consequences: because of the absence of cylindrical symmetry, double bonds cannot rotate (hence the Z/E isomerism), and because a π bond is weaker than σ bond, double bonds are not twice as strong as single bonds.

This gives us a basis to tackle chemical reactions. Indeed, double bonds and negatively charged sites are the main electron donors, whereas single bonds are more difficult to break, and so are unlikely to break and yield their electrons. Common electron acceptors include incomplete valence shells and positively charged sites. The curved arrow formalism can be introduced at this point, with simple examples from acid-base reactions, because such reactions are tackled in Lycée.

To conclude and give further illustrations of reaction mechanisms, Fischer esterification can be presented. It has the advantage of pointing out that curved arrows are indeed a *formalism* and not a *theory*, as they may be used to explain a reaction but hardly to predict it.

CONCLUSION

Although we cannot expect Seconde students to be fully familiar with even a real and stationary version of Quantum Mechanics at the end of a two-week internship, it appears possible to introduce them to the formalism of the theory, and use it to derive a simple (but quantum) picture of chemical bonds, molecular orbital theory and even chemical reactions.

Moreover, it was the occasion to introduce a number of concepts (quantum states, superposition, etc.) quite useful when the interns were to discuss with other researchers of the Laboratory, allowing them to understand at least the main ideas of their research.

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[3] G. N. Lewis, The atom and the molecule, Journal of the American Chemical Society **38**, 762 (1916).