van Quantum tot Molecuul

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Justification for the revised Course Guide

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1 Introduction and general context

In this document I present a detailed **justification of the redesign of the study guide** of the *"van Quantum tot Molecuul"* ("from quantum mechanics to molecules") course, offered to the second year students of the Bachelor in Medical Natural Sciences (NMW) at the VU. In particular, I provide a detailed justification of the various factors that have lead to the course redesign, including **situational factors** such as:

- The main reasons for the course redesign.

- The improvements that have been made, taking also into account student feedback.

- Who are the students, and what is their knowledge, their background, their interests and motivation.

- What part of the larger educational aims does the course contribute to.

- Why is the present course redesign a good means in realizing these aims.

- What is the place of the course in the larger educational setting at the VU, and how does this course connect to the previous and next courses.

- How does this course fit to the educational vision of the university.

In addition, I also provide a justification of the **revised course objectives**, covering important topics such as:

- Which course goals am I striving for? Why the choice of these specific goals?

- How can I contribute best to the academic development of the students, in a way that they can improve their critical and scientific thinking and complex problems solving skills?

In the third part of this justification, I consider the specific **teaching methods** adopted, addressing important issues such as:

- How did I structure the course?

- What and why is the order of the course components?

- How is the learning material distributed over the various course elements?

- What methods did you choose and why?

- Which learning activities do you use?

- Are the chosen teaching methods well adapted to the course objectives and the assessment methods?

Finally, in an appendix to this document I discus some more details of the **students learning using a castle-top sheet format**, addressing in particular how do I plan students learning before, after and in between the lectures.

In this respect, my BKO assignment is thus composed of:

- *The revised course study guide.*

- *The justification for the revised course guide* (this document). Here I also include a *castle-top sheet* that shows how the flow of in class and out of class activities is structured.

- *Two detailed lesson plans.*

- *an assessment plan, including the actual assessment and an answer model sheet.*

In order to complement the assignment, I also include attached to this justification and to the revised guide a number of appendices that will provide further information to evaluate my *Basisonderwijs Kwalificatie* including:

- *Original course study guide* (in Dutch).

- *Lecture notes (handouts) for some of my lessons of the course.*

- *Slides of the introductory lesson of the course.*

- *Slides of the presentation "Assessing, Testing, and Evaluating"* given on the 5th of October 2017.

- *Handout for the presentation "Assessing, Testing, and Evaluating".*

2   Situational factors

We begin this justification of how I have revised the course guide by discussing the corresponding situational factors, starting by which is the background of the students that follow this course and then moving on the improvements that have been carried out in order to tackle the existing limitations of the previous course design.

2.1   Students and background

The *"van Quantum tot Molecuul"* ("from quantum mechanics to molecules") course is part of the Bachelor in Medical Natural Sciences (*Medische Natuurwetenschappen*, MNW) offered by the VU:

http://www.bachelors.vu.nl/nl/opleidingen/medische-natuurwetenschappen/index.aspx

and is typically taken by second-year students. This is a recently started Bachelor course which aims to prepare students for a career related to applications of natural sciences (physics, chemistry and biology) into the medical world. Examples of career paths followed by students of this Bachelor in previous years include the design and realization of novel medical imaging tools (Magnetic Nuclear Imaging, Positron therapy) and guiding and organizing a hospital research laboratory.

One of the characteristic features of this Bachelor course is that the students come from very different backgrounds. Specifically, they have rather different preparation in important subjects like physics and mathematics. This is an important consideration to take into account in the course redesign, specially in order to avoid assuming any previous mathematical knowledge that the students might not have. On the other hand, their backgrounds in biology and chemistry are rather more similar.

The courses in the Bachelor in Medical Natural Sciences are usually taught in Dutch. This also means that part of the students are not fully comfortable receiving a lecture in English, and would rather prefer Dutch. Since I had to teach the course in English, I made clear from the beginning that all written assignments (such the the exercises during the tutorial sessions and the exams) as well as the communication with the course instructors and the teaching assistants could be carried out in Dutch language without any problem. So with the exception of the lectures that were in English, the students could choose to carry the rest of the course activities un Dutch if they felt more comfortable with that option.

Concerning the number of students, every year around 70 students start in the first year, with a man to woman ratio of 40%/60%. Since some students have to re-take some of the

courses, it is not unusual that for some of the most difficult courses more than 100 students are enrolled and attend regularly the lessons, requiring scheduling only lecture rooms that have the appropriate capacity.

The specific course selection that the students can follow is rather flexible, and is tailored in an individual basis in order to best suit the specific needs of each student. These course itineraries are organized around three main lines. The first one is for students that aim to be *scientifically driven*, and is focused on the study of chemical and physical processes in the human body to improve the understanding life and health. The second line is for those students that aim to be *clinically driven*, and is focused on applying chemical and physical understanding for better medical diagnosis and therapy. The third and final line is for those students that strive to be *societal driven*, concentrating on meaningful and economical medical care.

Within these three main lines, further specialization is also possible, including topics that range from Research, Communication, Education and Social, Forensic Science, Cardiovasculair research, Bio-informatics and systems Biology, Biomoleculair Sciences, Management, and Policy-Analysis to Entrepreneurship and Oncology.

2.2   Embedding in overall educational context

The VU aims to offer their students a broad range of courses, in most cases with a smooth connection with the professional world. In this respect, the nearby presence of the VU Medical Center (VUmc) makes the VU courses oriented towards life sciences topics specially strong and well-motivated.

In this general context, in the recent years a collaboration between different departments (including my own one, the Department of Physics and Astronomy) coordinated to create the new Bachelor in Medical Natural Sciences. The main aim of this Bachelor is to train students to follow a career in medical sciences, understood as professionals working in a medical environment (such a laboratory or a hospital) but that are focused on tasks different as those of doctors, such as in the design and fabrication of medical imaging and analysis equipment, or its operation in a day-to-day basis.

With this motivation, the overall aim of the *"van Quantum tot Molecuul"* course is to introduce the students to the basic mathematical language required to describe atoms, electrons, and molecules, by means of the quantum mechanical description of matter. On the one hand, this is required to gain a better understanding of the physical basis of important chemical properties and reactions frequently used in medical science. On the other hand, this

formalism allows us to translate quantum mechanical concepts into measurable quantities that can be used for medical applications, such as positron therapy or magnetic nuclear resonance. So it is a course that aims to bridge the gap between *fundamental concepts in the quantum theory of nature* and the *design and operation of medical tools and equipment* that rely on the exploitation of such quantum properties.

Specifically, the course starts with a gentle introduction to the quantum world, relevant for the description of small objects like atoms, molecules, and electrons. This will require presenting crucial concepts such as the wave-particle duality, the De Broglie relations, and the Heisenberg uncertainty principle of quantum mechanics. We will then move to present the fundamental equation of motion of quantum theory, namely the Schroedinger equation, and apply it to a number of important systems such as the particle in a box, the hydrogen atom, the harmonic oscillator, and the hydrogen atom. The course will explore next how quantum theory allows describing the binding mechanisms between atoms that lead to the formation of molecules, describing in particular the valence bond theory, the molecular orbital theory, the concepts of hybridization and molecular interactions, hydrogen bridges, and then Huckel theory. The last part of the course will consider molecular spectroscopy, with emphasis on its medical applications, and we will end up describing the underlying physics of one of the most popular tools in medical imaging, namely Nuclear Magnetic Resonance (NMR), illustrating the deep connection between the quantum description of nature and recent breakthroughs in medical science and tools.

Therefore, we can see from this brief summary that this course is special in that it covers a rather large amount of material from very fundamental for very applied topics. It is therefore essential to design the course ensuring that all students can follow the various topics covered in the course, from the most mathematically-oriented to the most applications-oriented students.

2.3   Reasons for the course redesign

I taught this course for the first time between January and March 2017. I replaced a fellow lecturer of my department who could not give the course due to illness. The course was originally taught in Dutch, so part of my duties were to translate in English the relevant material, including part of the syllabus and the study guide. I used this opportunity to improve the original course guide (see attachment), which was not as complete and comprehensive as it should be. In addition, I implemented many of the new concepts that I have learned during the present BKO course, and that have helped me in improve my course planning and

design skills. This has been a very profitable effort, since I might teach the course again in the next years, and so the attached revised course guide will become then the official course guide.

When I taught this course earlier this year, I noticed a number of problems with how the way was organized and taught, and that would require a number of important improvements:

- In the previous years, the instructors (lecturers) used power-point slides for all their lectures. I believe that from the pedagogical point of view this approach was not the optimal one for two main reasons. The first one is that the slides were really packed (with around 40 and 50 slides per lecture) so the risk was going too fast in most of the topics.

  The second criticism is that for many of the lectures the topics to be covered consisted of mathematical derivations, that are more easily digested by the students if carried out in the blackboard. Indeed, there is ample research showing that for more fundamental courses such as this one using the blackboard helps a lot to communicate the most important concepts to the students, rather than using slides.

- There was a confusing mix between theoretical concepts and practical examples. To be precise, sometimes too much time was devoted to practical examples without enough time devoted to the theoretical background concepts. This lead to the fact that most practical examples were too complicated to grasp with the specific theory concepts that the students had learned, and thus they were not that useful after all.

  In this respect, it would appear a better option to use less examples but better explained and with more time, and moreover connected better with the relevant theoretical concepts.

- The lectures were quite intensive: each lecture lasted 2 hours, with only a break of 10 minutes in the middle. Despite this heavy workload, there were no intermediate activities planned in order to keep the students engaged and motivated. This in general can cause that most of the students lose interest or lose track of the lecture contents halfway between the lecture. When lectures are that long, it is very important to design short activities to make sure that the students follow properly the whole lecture content until the very end.

- The course had a strong separation between the theory concepts (which were covered by the instructors on the *horscolleges*) and the practical ones (covered by the teaching

assistants in the *werkcolleges*). It was assumed that questions about the exercise sessions should be directed only to the TAs of the course, but not to the main instructors, and moreover, that during the main theory lectures no questions about the practical exercises was allowed.

This created an artificial separation between *theory* and *application* of the course concepts, and moreover did not allow to provide continuous feedback to the instructors about the progress of the students (since the exercise sessions were not part of the course assessment).

- The assessment of the course was limited to a partial exam, subsequently followed by a final exam. No other methods of assessment were accounted for, and in particular *no embedded assessment strategies* were considered.

  I believe this is a particular severe limitation for the practical exercise sessions: the students have to work for two hours on their exercises, supervised by their TAs, but this work does not have any influence on theory final mark, and is also never used in order to provide feedback to the instructors about how each student is performing.

In the next section, I present the improvements made in order to address the above limitations, applying both the concepts learned during this BKO course as well as the student feedback from previous years.

2.4   Improvements made and student feedback

As mentioned in the previous section, I realized that there were a number problems with way in how the course was organized and taught the previous years. Aiming to overcome these limitations, and accounting as well to the feedback received by the students in previous years, I have implemented the following modifications in the course design:

- To begin with, lecture handouts will be make available on Canvas well in advance of each theory lecture. This way students can concentrate on following the lecture contents without the need of taking their own notes, they can simply complement the material included in the handout.

  Examples of handouts that will be made available to the students are included in the appendices. These handouts contain all the material necessary to cover the course lectures, and in particular they reduce the need to digest the course textbook, which covers way more material than what corresponds to the actual course.

- To overcome the unnecessary complex mix between theory and experimental context, I have revised the course contents (including the material presented in the handouts) to weight more for the theory part and include only few selected, but highly representative, examples, which are then explained in detail. Moreover, the handouts point to further examples in the course textbook that the students can read by themselves if they find necessary.

  By concentrating on the theory foundations, the students are better prepared to study by themselves the corresponding practical applications.

- To make sure that the students remain motivated and attentive during the whole lecture, I will use the `Mentimeter` system

  https://www.mentimeter.com/

  in order to ask short questions to the students and monitor their replies. This also provides useful feedback to assess where one I should emphasize specific topics during the lectures, in particular those who are more difficult to grasp by the students. The latter goal is achieved by keeping an archive of questions and the output of the corresponding answers, which is easily done via this online tool.

- As mentioned above, in previous installments of the course the students had to attend compulsory tutorial sessions (*werkcolleges*) where they were supported by the teaching assistants, but their work did not contribute to the final assessment.

  In the course redesign, I have included that the students will need *to carry out two specific exercises per tutorial session* (in addition to the rest of the exercises) which will be marked by the TAs an contribute to the final grade. This realizes the idea of *embedded assessment*, where activities that the students need to carry out anyway as part of the teaching becomes now also integral part of the assessment of the course. The work performed during the exercise sessions counts 25% towards the final mark of the course, as discussed in the revised study guide.

- A major problem of how the course was previously organized is that the instructors did not received any feedback about the student progress until at least the partial exam, and this could be too late in some cases.

  Exploiting the previous measure (TAs marking some of the problems that the students) also solves this problem, since each student will be marked by their work in the tutorial

session, and this will provide the instructors with very valuable information in order to fine tune the contents of the subsequent lectures.

All these measures have been implemented in the revised course guide, attached to this document.

Concerning the student feedback, perhaps the most recurrent complain was that they found very useful to have detailed high-quality lecture notes provided to them in advance. This way they could read and print them beforehand, and concentrate during the lecture in following what I was explaining rather than on note taking. This was beneficial for their performance, since ample research shows that a large fraction of the class notes taken by university students is of rather low quality. As mentioned above, I will provide detailed handouts for each the course lectures, and I have provided some examples of handouts in the appendices of this assignment.

Another usual feedback provided by the students was due to the fact that the final grade was constructed only based on the partial and final exams, and that there were no in-class or out-class activities that they could carry out to complement the course assessment. This was specially problematic since some of the students following this course had an inferior background in mathematics, and therefore they required more time to carry out the exercises as compared to other students. This makes difficult for them to perform well in an exam, and extra time to carry out the activities would help them a lot. To address this feedback, as mentioned above, now 25% of the total course grade is provided by the exercises carried out during the tutorial sessions, which is moreover a rather more relaxed environment than the actual exams.

2.5   Place of the course within the VU

Next we discuss what is the place of the course in the larger educational setting at the VU, and specifically how does this course connect to the previous and next courses.

The course *"van Quantum to Molecuul"* is one of the central courses of the Bachelor degree in Medical Natural Sciences, which aims to prepare students to follow a career in professions that combine Physics, Chemistry, Math, Computer Science and Physiology in a medical context. The ultimate goal is to develop an understanding of scientific and technical state of the art in medicine. In this respect, it is a unique program in the Netherlands higher education ecosystem. Moreover, thanks to the direct cooperation between the VU Science Faculty and VU Medical Center, this bachelor degree is located entirely at the VU campus.

The career paths that the students can follow afterward are very varied. These include jobs in in research (both in academia and in medical clinics), health sciences, or industry (in companies such as TNO, Philips or Medtronic). For example, a recent survey of the career paths followed by students of the MNW bachelor degree indicate that 75% had a job only three months after their graduation, while 90% had a job after 6 months of their graduation. In addition, many of the students continue their higher education by transferring to a related master course, such MNW MSc or the Physics of Life track of the MSc in Physics and Astronomy. From there on, a small fraction of students continue their higher education studies to perform a PhD degree.

One of the main difficulties in teaching this course, which is also important to the general context, is that specially physics lecturers find that students have *poor math skills*. This has lead to an effort to uniformize the math content of the various courses that compose the MNW bachelor degree. Specifically, some *foundation* courses are offered for the students that want to improve their level of mathematics and physics before moving to the rest of courses in the degree.

3   Revised course objectives

Next we turn to present the revised course objectives, and the reasons why the have changed them as compared to the original ones.

3.1   Motivation of choice of specific course goals

As can be read from the revised study guide, now each lecture (*horscollegen*) has a well-defined set of learning goals. These learning goals summarize the most important concepts that the students should grasp after each lecture. The specific choice of the learning objectives for each lecture is motivated by the following criteria:

- The students should attain a sufficiently proficient understanding of the basic concepts of Quantum Theory, including being able to perform calculations in important systems such as the quantum harmonic oscillator and the hydrogen atom.

- The students should be ably to apply this acquired knowledge in order to understand and interpret physical phenomena of direct relevance to the practitioners of Medical Natural Sciences, such as the different types of molecular spectroscopy or how to identify organic molecules based on specific radiation patterns.

- The students should be able to understand both the physical and technological under-pinnings of the most important techniques of medical imaging, treatment, and analysis, and to connect them with the fundamental concepts of the quantum theory of Nature. These include Magnetic Nuclear Resonance, Positron Therapy, or cancel therapy using photosensitive molecules, among several others.

Based on these considerations, the *revised list of main course goals* (also listed in the revised version of the study guide) are the following:

- Understand why the Quantum Theory is necessary to describe the structure and properties of electrons, atoms and molecules, and in which respect it represents a radical departure with respect to the intuitive concepts of classical physics.

- Understand how experimental observables can be calculated from the quantum wave-function as a solution of the Schrödinger equation with different symmetries and boundary conditions, and perform these calculations in simple systems.

- To able to determine the electronic structure of the hydrogen atom in terms of electronic levels and shells, in particular taking into account the role of angular momentum, by means of solving the Schrödinger equation in systems with rotational symmetry.

- To be able to derive solutions for the Schrödinger equation for multi-electron atoms by means of the orbital approach, and to determine in which respect the resulting electronic structure differs from that of the hydrogen atom.

- To become familiar with the concept of molecular orbital, and to be able to represent it in terms of the underlying probability density. This goal also involves being able to combine electric orbitals from individual atoms into joint molecular orbitals.

- To understand the basic symmetry properties of molecular orbitals, with special emphasis on the role of angular momentum, and to be able to determine the resulting consequences for the electronic structure of important molecules.

- Understanding and applying the basic properties of absorption and emission of electromagnetic radiation in molecules, and being able to determine which specific properties of important molecules we can access which each type of radiative process.

- Understanding and applying the principles of fluorescence and phosphorescence, and being able to compute the rates of different radiative emission processes of relevant molecules.

- Become familiar with the basic principles of Magnetic Resonance Imaging, and understand how the spin of atomic nuclei represents one of the most helpful ingredients of modern medical imaging.

At the end of the course, the students should have achieved the skills and competences necessary to satisfactory consider these course goals as accomplished.

3.2   Contribution to academic development of students

One of the most important considerations that need to be taken into account when revising the objectives of a given course is what are the best strategies in order to contribute to the academic development of the students. Specifically, one needs to carefully think how the course objectives are going to improve their critical and scientific thinking abilities, as well as their skills for solving non-trivial problems.

As discussed above, the present course redesign has thoroughly addresses a number of flaws of the original design and implemented them in the revised course guide. Specifically concerning the contribution to the academic development of students, I would like to emphasize the following points:

- In the revised course planning, rather more weight is given to boost the *problem-solving abilities* of the students as compared to the original planning. This is now achieved by turning the tutorial sessions in which the students have to participate into a component of the course's embedded assessment. Since now the students will have two compulsory exercises to carry out per tutorial session, and these will count 25% of the total mark, students have a greater incentive to work hard on their problem solving skills, specifically practicing them before the tutorial session (since the students know beforehand the list of problems which will be covered in each tutorial session). Note that before the tutorial (problem-solving) sessions carried no weight in the final mark, so the students had less motivation to improve their problem-solving abilities.

- Their *scientific thinking abilities* will be improved since in the revised planning of the course the students will be exposed to careful physical derivations of important concepts by the lecturer on the blackboard, rather than merely being flashed busy slides with many formulas. By following the flux of the derivations, the students can visualize how the scientific progress works in practice from an initial set of hypothesis that end up after mathematical manipulation into a well-defined set of theoretical predictions than can be compared with the experiment.

The fact that the students will have access beforehand to detailed lecture notes ensures that they will be able to concentrate on the actual derivations being carried out by the lecturers rather than in their actual note-taking.

- The *critical abilities* of the students will be strengthened by the new set of in-class activities that I have scheduled, in particular those using the `Mentimeter` tool. Using this tool, which requires as input nothing more that the student's smartphone, I can carry out quick questions and polls during the class, both to keep the students engaged and to ensure that they have grasped properly a given set of concepts before moving to the subsequent ones.

  I will use the results of these quizzes to trigger short discussion between the students, where they need to explain why they have chosen a given answer, and if they got the wrong one, if now they understand why the correct answer was a different one. This kind of informal discussions about the topics covered during the lectures will certainly improve and enhance the *student's critical abilities*, motivating them to justify their answers and to explain their choices to their peers.

4 Choice of teaching methods

Now I move to motivate the choice of specific **teaching methods** adopted in the present course redesign.

4.1 Course structure and order

As discussed above, the aim of this course is to provide students that *aim to train for a career in the medical natural sciences* with the basic concepts of quantum theory that are required to design, understand, and operate medical analysis, treatment and characterization tools such as Magnetic Nuclear Imaging, Photosensitive Therapy and Positron Therapy.

Given this aim, the course is structured as a *learning process* that builds from the *basic concepts of quantum theory* up to the practical operation of *advanced medical equipment*. Therefore, the order and the structure of the course is dictated by the fact that before moving to a new topic the students should be confident with the topics of the previous lectures. This is perhaps rather different to other courses, where each lecture is more of a *self-consistent unit*.

To illustrate these deep interconnections of the various components of the course, that call for a well-organized structure, let me highlight the interplay between the subsequent course contents (see also the *Revised course guide*):

- We start by introducing the basic concepts of quantum theory such as the quantum wave function and the Schroendiger equation.

- We then use these theoretical concepts to start to learn how to carry out simple calculations in quantum theory, such as the *particle in a box*.

- Building upon this simple cases, we move to apply Schroendiger equation to more complex cases of direct physical interests, specifically the hydrogen atom.

- Once the students have become familiar with the hydrogen atom, we move to move complex atoms based on more than one electron, and determine how the resulting electronic structure is modified.

- Moving towards more advanced topics, we leave behind individual atomics and move to molecules, applying the techniques learned before to the calculation of electronic levels there.

- There any many different possible transitions between energy levels in molecules, so now we need to separate the various classes and understand what are their observational tell-tale signatures.

- Finally, the students have to combine all what they have learned during the course in order to understand the underpinnings of crucial applications of medical natural sciences such Magnetic Nuclear Imaging, Photosensitive therapy and positron therapy.

This specific choice of course structure guarantees a *smooth transition of the learning curve of the students* from the more basic, conceptual topics to the more advanced topics such as the operation and manipulation of medical imaging and treatment tools.

4.2   Choice of teaching methods

During the theory lectures, I will use the *blackboard* as the main teaching method. The reason is that this is a course which is based mostly on mathematical derivations, where starting from a given set of physical laws and requirements we need to work out the solutions of different problems. I firmly believe that in this respect the use of *blackboard* is highly preferable upon

other methods such as power-point slides, which tend to accumulate too much material in too little space, and moreover then then to be covered too quickly for the student to properly digest all the comments.

As an additional benefits, thanks to the movable blackboards which are available in most of the VU classrooms, it is possible to write everything that is needed into a single lecture on the blackboard while having to erase it at most one or twice during the lecture. This is most useful, since this way the students can go back at the previous steps of the derivation, at graphs that I have drawn etc, facilitating that they get the *full picture* of the topics that are being discussed in each lecture.

One could argue that this choice of teaching method is non-optimal since the students are then forced to take notes during the class, which are known to be usually of low quality. This concern does however do not apply in this case, since detailed lecture notes will be provided before each lecture on **Canvas**. This way the students only need to annotate the lecture notes with their own comments and personal notes, but they don't need to worry i.e. of copying all the equations from the blackboard to their notepad.

4.3   Choice of learning activities

The *learning activities of this course* (see also the Appendix) can be divided into *in-class activities* and *out-of-class activities*. The former include the theory lectures, the problem-solving tutorial sessions, as well as short quizzes or group work within the lecture (see *Lesson Planning*). The latter include the preparation for the lecture reading the lectures notes as well as other materials such as the textbook and videos, the preparation of the problems to be carried out during the tutorial sessions, and the revision of the complete course material both before the partial exam and then after the partial exam.

This specific choice of learning activities aims to maximize the usefulness of the course for the students in order to achieve the *course objectives*. Moreover, it provides a suitable balance of complementary learning activities, whose combination contributes to enhance and facilitate the *student learning*. In particular:

- The theory lectures provide the necessary *foundations* to understand the consequences of applying the principles of quantum theory to natural medical sciences.

- The tutorial sessions are tailored to enhanced the *problem-solving skills* of the students, as well as to ensure that they have properly interiorised the concepts presented during theoretical lectures.

- The short in-class activities such as polls, quizzes, and group work helps to both keep the students *engaged* during the full duration of the lecture as well as to provide useful *feedback* for the structures about the learning performance of the students.

- The preparation of the lectures and the tutorial sessions ensures that students do not start them like a *tabula rasa*, specially since they have at their disposal the complete set of lecture notes and of problem sets.

- The revision of the whole course material for the exam is an essential preparation for the most important part of the *course assessment*, and is facilitates by the prevision of exams (together with their solutions) from previous years.

A   Castle-top representation of course activities

In this appendix I present a graphical representation of the various course activities using the *castle-top format*. It is divided between *in-class activities*, to be carried out in the lectures, and *out-of-class activities*, to be carried out by the students between the lectures, and include as well the preparation of the exercises for the tutorial sessions. Following this, I provide some explanations related to how specifically do I plan students learning before, after and in between the lectures.

van Quantum tot Molecuul
Castle-top Summary of course activities

	HC1		HC2		HC2	
In class Activities	Course introduction. Presentation of assessment methods. Overview of quantum theory		Schroedinger equation. Interpretation of the wave function.		Heisenberg's uncertainty principle. Particle in a box. Quantum harmonic oscillator.	
Out of class Activities		Prepare exercises for the tutorial session. Watch videos avoid historical origin of quantum theory		Prepare exercises for the tutorial session.		Prepare exercises for the tutorial session.

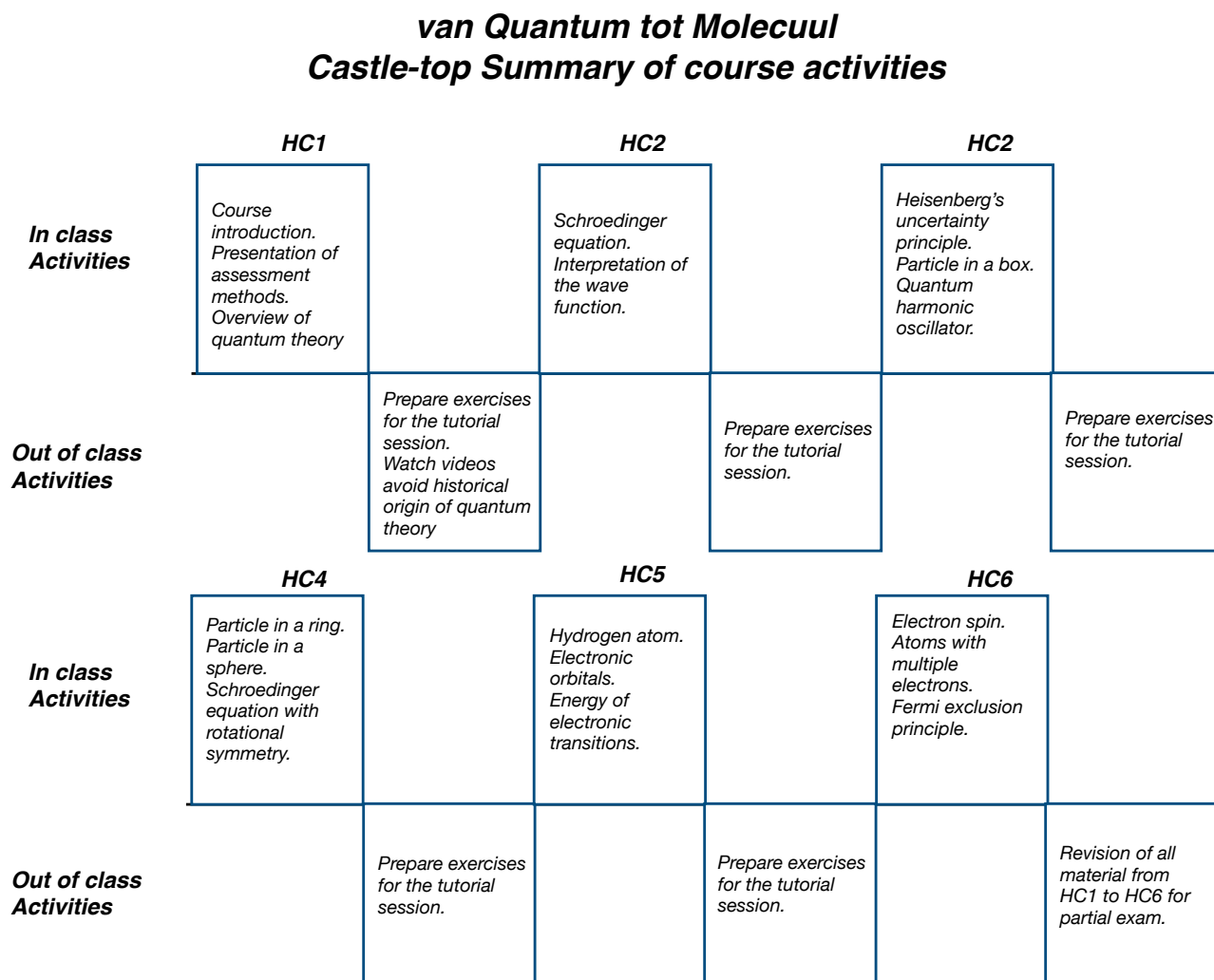|	HC4		HC5		HC6	
In class Activities	Particle in a ring. Particle in a sphere. Schroedinger equation with rotational symmetry.		Hydrogen atom. Electronic orbitals. Energy of electronic transitions.		Electron spin. Atoms with multiple electrons. Fermi exclusion principle.	
Out of class Activities		Prepare exercises for the tutorial session.		Prepare exercises for the tutorial session.		Revision of all material from HC1 to HC6 for partial exam.

Figure A.1: Graphical representation of the various course activities using the castle-top format.

As indicated by the castle-top structure of the course the student learning takes place both during the *in-class activities* and the *out-of-class activities*. Specifically, in each type of activities we have the following:

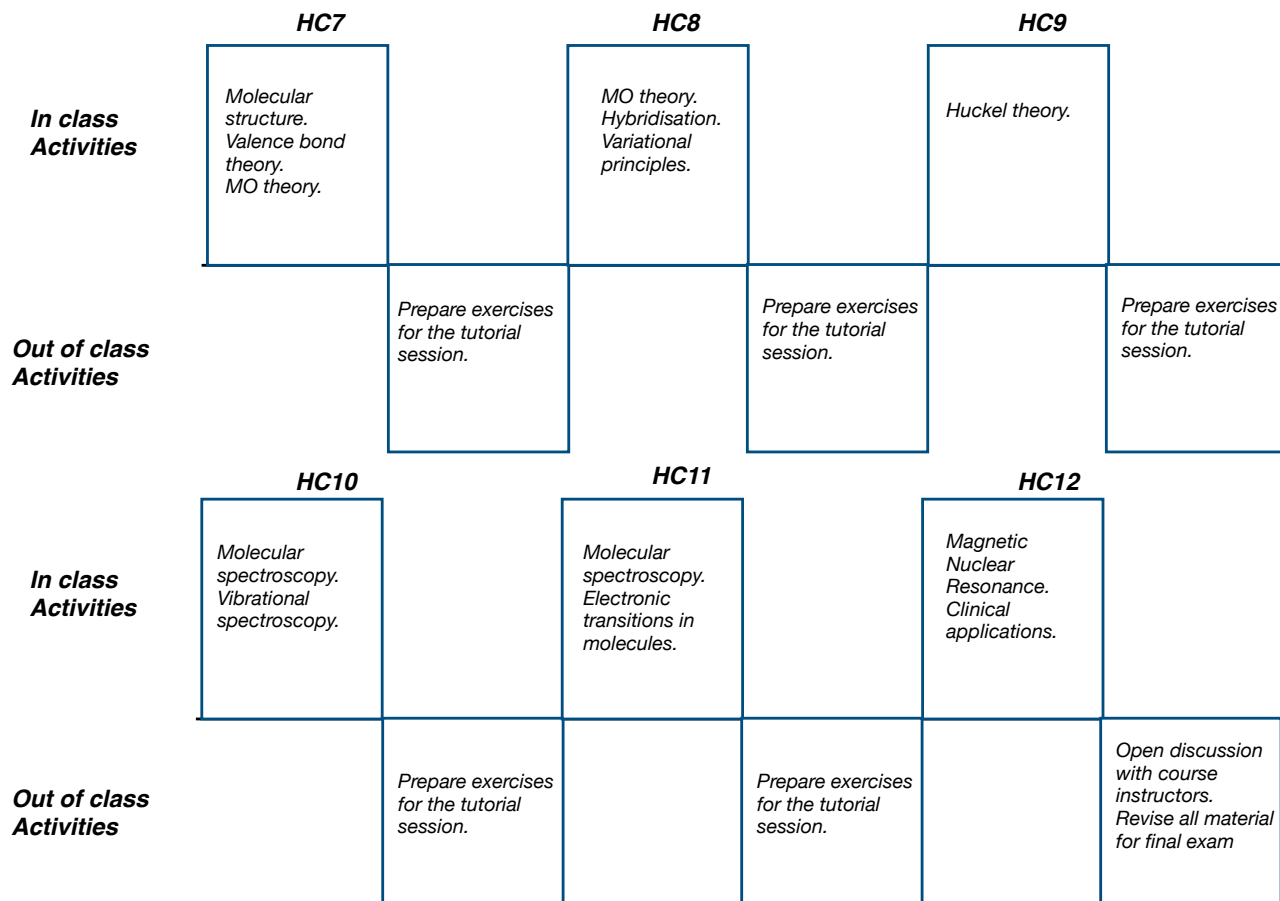## van Quantum tot Molecuul
Castle-top Summary of course activities

	HC7		HC8		HC9	
In class Activities	Molecular structure. Valence bond theory. MO theory.		MO theory. Hybridisation. Variational principles.		Huckel theory.	
Out of class Activities		Prepare exercises for the tutorial session.		Prepare exercises for the tutorial session.		Prepare exercises for the tutorial session.

	HC10		HC11		HC12	
In class Activities	Molecular spectroscopy. Vibrational spectroscopy.		Molecular spectroscopy. Electronic transitions in molecules.		Magnetic Nuclear Resonance. Clinical applications.	
Out of class Activities		Prepare exercises for the tutorial session.		Prepare exercises for the tutorial session.		Open discussion with course instructors. Revise all material for final exam

Figure A.2: Graphical representation of the various course activities using the castle-top format (continued).

- The *in-class activities* are focused on presenting the various theoretical concepts as well as the corresponding practical applications. In this learning, the students are supposed by detailed *lecture notes* (see Appendices) which are made available in **Canvas** before each lecture.

  In addition, as discussed in some detail in the *Lesson Planning* document, during the lectures there are additional short in-class activities such as *polls, quizzes, and group-work* that are important both to keep the students engaged and to provide feedback to the instructors about how well they are achieving the various course learning objectives.

- The *out-of-class* activities include mostly the *preparation for the exercises* to be carried

out during the tutorial sessions. In this aspect of their learning, the students are supported by the lecture notes, the list of exercises provided beforehand, as well as by the *course textbook* that provides additional material for students that want to delve deeper in some specific topics.

Here an important consideration is that some of the problems that the students are expected to carry out come together with their *numerical answer*. This provides a further help to the students since, already before the tutorial sessions, they can check which problems they solve correctly and in which problems they are stuck. This way during the tutorial sessions the TAs can focus on addressing the *most challenging aspects of the student learning*, rather than those that have been already properly digested and that do not require spending extra time on them.

Other important out-of-class activities that are indicated in the castle-top diagram include *watching videos about the historical origin of quantum theory* (which we provide, and that provide a good motivation to the specific choice of course learning objectives), the *revision of the course material* in preparation first for the partial exam, and then for the final exam, and the *open discussion session* with the course instructors, that takes place just before the final exam and provides a good opportunity for the students to discuss pending urgent questions.

Finally, it should also be considered in the category of *out-of-class activities* the office hours with the course instructors. As specified in the *Revised study guide*, the instructors are available up to 30 min after each lecture in order to answers any course-related questions from the students. Moreover, additional office contact hours can be arranged by email when required.

The combination of planned *in-class* and *out-of-class* activities then provides a suitable balance to assist and support the *student learning* from a combination of classroom activities and of work that the students are expected to do on their own or together with their peers. To summarize these justification, let me recapitulate how in this course redesign I have planned to *assist student learning before, after, and in between the lectures*:

- **Before the lectures**: the students should read the lecture notes posted on **Canvas** as well as additional reading material (textbook) and visual material (videos) to prepare the lectures.

- **In between the lectures**: the students should read again the lecture notes, this time with their own notes taken during the lecture, and *reflect* about what they have

learned in the process. The students should also prepare the *tutorial sessions* by using the concepts learned during the lectures, and using the help from the teaching assistants to clarify the most difficult concepts.

- **After the lectures**: the students should revise all the course materials (lecture notes, textbook, exercises) in preparation for the exams. The instructors are available then to discuss any outstanding question with the students.

van Quantum tot Molecuul

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Revised Course Guide

current version: October 19, 2017

Staff Developer: Dr Anja Swennen

Tutor: Prof Piet Mulders

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Van Quantum tot Molecuul
STUDY GUIDE

1   General context

The *"van Quantum tot Molecuul"* ("from quantum mechanics to molecules") course is part of the Bachelor in Medical Natural Sciences (*Medische Natuurwetenschappen*, MNW) offered by the VU:

http://www.bachelors.vu.nl/nl/opleidingen/medische-natuurwetenschappen/index.aspx

and is typically taken by second-year students. The overall aim of this course is to introduce the students to the basic mathematical language required to describe atoms, electrons, and molecules, by means of the quantum mechanical description of matter. On the one hand, this is required to gain a better understanding of the physical basis of important chemical properties and reactions frequently used in medical science. On the other hand, this formalism allows us to translate quantum mechanical concepts into measurable quantities that can be used for medical applications, such as positron therapy or magnetic nuclear resonance.

Specifically, the course starts with a gentle introduction to the quantum world, relevant for the description of small objects like atoms, molecules, and electrons. This will require presenting crucial concepts such as the wave-particle duality, the De Broglie relations, and the Heisenberg uncertainty principle of quantum mechanics. We will then move to present the fundamental equation of motion of quantum theory, namely the Schroedinger equation, and apply it to a number of important systems such as the particle in a box, the hydrogen atom, the harmonic oscillator, and the hydrogen atom.

The course will explore next how quantum theory allows describing the binding mechanisms between atoms that lead to the formation of molecules, describing in particular the valence bond theory, the molecular orbital theory, the concepts of hybridization and molecular interactions, hydrogen bridges, and then Huckel theory. The last part of the course will consider molecular spectroscopy, with emphasis on its medical applications, and we will end up describing the underlying physics of one of the most popular tools in medical imaging, namely Nuclear Magnetic Resonance (NMR), illustrating the deep connection between the quantum description of nature and recent breakthroughs in medical science and tools.

2   Lecturers and teaching assistants

The two lecturers (*docenten*) of the course are

Dr. Juan Rojo

Kamer T230 Wis- en Natuurkundegebouw

Tel. 020-5987212

j.rojo@vu.nl

and

Prof. Dr. Ir. Erwin Peterman

Kamer U022, Wis- en Natuurkundegebouw

Tel. 020-59 87576

e.j.g.peterman@vu.nl

In addition, the tutorial sessions (*wercolleges*) will be supervised by three teaching assistants (*assistenten*):

- Veerle Brans (v.a.brans@student.vu.nl)

- Luuk Geelen (l.h.c.geelen@student.vu.nl)

- Margherita Marchetti (m.marchetti@vu.nl)

The material covered in this course follows mostly the content of the course textbook, *Physical Chemistry* by Atkins & De Paula (10th edition, Oxford University Press). Note that previous editions have a different chapter structure, so we strongly recommend the students to buy the latest edition (it can be acquired at the VU bookshop).

In addition to the textbook, lecture notes for each of the HCs and additional learning materials can be found in the Canvas page of the course, as well as here:

http://juanrojo.com/teaching

3   Course schedule

The detailed course schedule, including the division between lectures (*horscolleges*) and tutorial sessions (*wercolleges*), is indicated in Table 3.1. There we indicate the date and time

Week	Dag	Datum	Tijd	HC/WC	Docent	Topic
2	Ma	9-1	13:30	-	JR	GEEN COLLEGE
2	Di	10-1	13:30	HC1	JR	Overzicht cursus, introductie quantum, Ch 7
2	Vr	13-1	11:00	WC1		WC1
3	Ma	16-1	13:30	HC2	JR	Ch 7: Schrodinger vergelijking, interpretatie vd golffunctie, wiskundig gereedschap
3	Di	17-1	13:30	HC3	JR	Ch7: Heisenberg onzekerheidsrelaties Ch 8: vrije deeltje, deeltje in 'n doosje, tunneling, harmonische oscillator
3	Vr	20-1	11:00	WC2		WC2
4	Ma	23-1	13:30	HC4	EP	Ch 8: Deeltje op 'n ring, deeltje op 'n bol
4	Di	24-1		HC5		Ch 9: waterstofatoom
4	Vr	27-1	11:00	WC3		WC3
5	Ma	30-1	13:30	HC6	EP	Ch 9: electronspin, meer-electron atomen
5	Di	31-1		HC7	EP	Ch 10: moleculaire structuur, valence bond theorie, MO theorie,
5	Vr	3-2	11:00	WC4	TAs	WC4
6	Di	7-2	13:30	WC5	TAs	WC5
6	Vr	10-2	11:00			GEEN COLLEGE
7	Di	14-2	13:30			GEEN COLLEGE

Week	Dag	Datum	Tijd	HC/WC	Docent	Topic
7	Vr	17-2	11:00			TUSSENTOETS
8	Di	21-2	13:30	HC8	EP	Ch 10: MO theorie hybridisatie, variatieprincipe
8	Vr	24-2	11:00	HC9	EP	Ch10: Hückel theorie
9	Di	28-2	13:30	WC6	TAs	WC6
9	Vr	3-3	11:00	HC10	JR	Ch 12: moleculaire spectroscopie, vibrationele spectroscopie
10	Di	7-3	13:30	WC7	TAs	WC8
10	Vr	10-3	11:00	HC11	JR	Ch 13: moleculaire spectroscopie, electronische overgangen
11	Di	14-3	13:30	WC8	TAs	WC9
11	Vr	17-3	11:00	HC12	JR	Ch 14: NMR
12	Di	21-3	13:30	WC9	TAs	WC9
12	Vr	24-3	11:00	VRAGEN	JR/EP	VRAGENUUR
13	Di	28-3	15:15-18:00			TENTAMEN

Figure 3.1: Course schedule. For each entry in the table we indicate the semester week, the date and time of the lecture, the type of lecture (full lecture or tutorial) and the name of the instructor. We also provide a short description of the topics that will be covered in each lecture, where the chapter numbers correspond to the course textbook (Physical Chemistry, Atkins & De Paula, 10th edition). The dates of the intermediate and final exams are also listed here.

where the lecture will take place, the names of the instructor, and the specific topics that will be covered during the lecture. The dates of the intermediate and final exams are also listed here (see below for more information about the course assessment). Note that the specific lecture rooms can be found by logging into Canvas and going to the *"van Quantum tot Molecuul"* course page. You should all have received an invitation to join this course on *Canvas*, else please contact the course instructors and they will try to assist you.

We emphasize that the course have been designed so that the content of each lecture depends heavily on those concepts and topics covered in previous lectures. Therefore assistance to all the lecture sessions, while not compulsory for the course assessment, is strongly encouraged. If you are not able to attend some lectures, note that some of them will have been recorded and made available afterwards.

4   Course assessment I: partial and final exam

The assessment of this course is divided into two separate parts: (i) two tests, one around halfway of the course and the second at the end of the course, and (ii) the participation in the tutorial sessions with the teaching assistants. We present here the details of these examinations, and in the next section we discuss how the tutorial sessions will be organized.

- There will be first an intermediate examination towards the end of the first half of the course (*tussentoets*) followed by a final test at the end of the course, once all the lectures and tutorial sessions have been carried out (*volledig eindtentamen*).

- The date and time of the partial exam, the *tussentoets*, is Friday 17th February 2017, 11am. The material that will be covered includes everything from the start to the course to the topics covered in HC6, inclusive (see Table 3.1 and the detailed course syllabus below).

- The date and time of the final course exam, the *voledig tentamen*, is the Tuesday 28th March 2017, 3.15pm. This final exam will contain two parts, the first of all covering the same content as the partial exam (Part I, covering from HC1 to HC6 inclusive) and then a second part covering the remaining of the course materials (Part II, covering from HC7 to HC12 inclusive).

- Whether or not an student needs to carry out both Parts I and II of the final exam depends on the marks that she obtained during the partial exam (*tussentoets*). Specifically, if the grade obtained in the intermediate exam was insufficient, the complete final exam needs to be performed (Parts I+II). On the other hand, if the grade obtained in the exam is a pass or higher, there is the option to either skipping or attempting Part I in the final exam. In the latter case, the best of the two marks will be the one that counts for the course evaluation

Note that both during the partial and the final exam, the use of any external material such as textbook of formulae lists is not allowed. Likewise, the use of scientific programmable calculators us not allowed: the students are allowed to bring only a simple calculator without memory for mathematical expressions. Together with the exam, a list of potentially useful physical equations, mathematical relations and physical constants will be provided to the students.

An important remark concerns the students re-taking the course after they have failed in the previous years. In this case, these students need to perform the complete final exam

(both Part I and Part II) unless they pass the intermediate exam during the same year. In other words, the marks from intermediate examinations cannot be carried forward from previous years. On the other hand, attendance to the tutorial sessions (*werkcolleges*) is not mandatory for those students that are re-taking the course.

5   Course assessment II: tutorial sessions

The second part of the course assessment is based on tutorial sessions. Indeed, a very important part of the course is the active participation of all the students in the tutorial sessions (*werkcolleges* in Dutch). In total there will be 9 of such tutorial sessions, and attendance to the tutorials is compulsory (else examination will not be allowed).

To demonstrate your attendance, it is important to you remember to write your name in the attendance list at the start and end of the tutorial session. Note that if, for a good reason such as illness or other unforeseen circumstances, you are not able to attend a specific tutorial session, please inform the Teaching Assistants by email before the start of the session that you will miss.

In this respect, in order to take the most profit of these tutorial sessions, it is very important that you prepare in advance the tutorial work for each session, taking into account the following guidelines:

- Read the corresponding chapters in the textbook and the lecture notes in advance, in order to become familiar with the basic concepts underlying the problems that will be carried out during the tutorial session.

- The exercises corresponding to each tutorial session will be announced in advance by the teaching assistants. If you have questions, you can also contact them via email either before or after the specific tutorial session.

- Self-organise yourselves in groups of three or four students to prepare beforehand the tutorial work for each session.

- Note that it is possible to submit specific questions by email about the exercises to the TAs at any point during the course, including about problems covered in previous tutorial sessions.

These tutorial sessions represent an integral part of the course, and we expect students to take them very seriously.

Moreover, these tutorial sessions contribute to 25% of the total grade, with the other 75% corresponding to the results of the partial and final exams. At the beginning of each tutorial session, the TAs will indicate two specific problems (out the entire list that had been indicated to you beforehand), which you will need to carry out and then hand in to the TAs. They will mark these problems, and the average mark our of the 9 tutorial sessions will then add up to 25% of the total course grade.

6   Communications

The main interface for the communications between the students and the instructors is the `Canvas` page for the course. All the relevant course documents and teaching materials will be make available there. It is important that you familiarize yourselves with `Canvas` if you have never used it before. You can fine many online tutorials describing the use of `Canvas`, such as for instance this one:

https://www.youtube.com/watch?v=bHyUPjf37rY

In particular, please take into account the following points concerning the communication of relevant course information:

- All the students registered in the course will receive automatically the course notifications via the `Canvas` interface. If you have any trouble receiving the emails, please contact the IT help-desk or the `Canvas` help-desk for assistance.

- The relevant information about the course, tutorial sessions, and evaluations and exams will take place though your VU student email. Therefore, please check regularly your VU email, at least once per day during term.

- It might be in your interest to configure a forward to the email account you check more frequently, in order to avoid the need to checking two accounts regularly.

- Note that changes in the course schedule such as different lecture rooms will be announced by email, so please be aware of possible last-minute changes.

7   Office hours

The lecturers will be available up to half an hour after each lecture to discuss open questions. Additional office hours can be scheduled via contacting per email the lecturers, and will take

place in their offices T231 (JR) and T054A (EP). As mentioned above, questions specific to the problems discussed in the tutorial sessions should be directed to the teaching assistants of the course rather than to the instructors.

8   Course objectives

At the end of this course, the students should be able to satisfactorily master the following set of course objectives:

- Understand why the Quantum Theory is necessary to describe the structure and properties of electrons, atoms and molecules, and in which respect it represents a radical departure with respect to the intuitive concepts of classical physics.

- Understand how experimental observables can be calculated from the quantum wavefunction as a solution of the Schrödinger equation with different symmetries and boundary conditions, and perform these calculations in simple systems.

- To able to determine the electronic structure of the hydrogen atom in terms of electronic levels and shells, in particular taking into account the role of angular momentum, by means of solving the Schrödinger equation in systems with rotational symmetry.

- To be able to derive solutions for the Schrödinger equation for multi-electron atoms by means of the orbital approach, and to determine in which respect the resulting electronic structure differs from that of the hydrogen atom.

- To become familiar with the concept of molecular orbital, and to be able to represent it in terms of the underlying probability density. This goal also involves being able to combine electric orbitals from individual atoms into joint molecular orbitals.

- To understand the basic symmetry properties of molecular orbitals, with special emphasis on the role of angular momentum, and to be able to determine the resulting consequences for the electronic structure of important molecules.

- Understanding and applying the basic properties of absorption and emission of electromagnetic radiation in molecules, and being able to determine which specific properties of important molecules we can access which each type of radiative process.

- Understanding and applying the principles of fluorescence and phosphorescence, and being able to compute the rates of different radiative emission processes of relevant molecules.

- Become familiar with the basic principles of Magnetic Resonance Imaging, and understand how the spin of atomic nuclei represents one of the most helpful ingredients of modern medical imaging.

9   Course syllabus

In the following we present the specific detailed syllabus of the course. As indicated in Table 3.1, the course is divided into 12 *horscollegen* (HCs), each one corresponding to a 2-hour lecture. For each HC, we present a general overview of the topics that will be covered and the specific *Learning Goals* of each lecture. We also indicate the corresponding chapters in the course textbook that will be covered in each lecture.

The 12 *horscollegen* of the course will cover the following topics:

- HC1: Introduction to quantum theory.

- HC2: The quantum wave-function and the Schroedinger equation.

- HC3: Quantum mechanics of simple systems.

- HC4: The Schroedinger equation for systems with rotational symmetry.

- HC5: The hydrogen atom.

- HC6: Multi-electron atoms and orbital theory.

- HC7: Molecular structure.

- HC8: Molecular Orbital theory and hybridization.

- HC9: Huckel theory.

- HC10: Molecular and vibrational spectroscopy.

- HC11: Molecular spectroscopy and electronic transitions.

- HC12: Magnetic nuclear resonance.

In the following, we detail the contents of each of these HCs in turn.

9.1   HC1: Introduction to Quantum Theory

General introduction to Quantum Theory

Based on Atkins and de Paula, *Physical Chemistry* 10th edition, Chapter 7

In this first lecture we provide a general historical introduction to the main theoretical and experimental development that culminated in the modern formulation of quantum mechanics, and present some of the most important concepts in quantum theory such as the intrinsic duality between waves and particles. This lecture is basically qualitative and historical, with the main goal of providing the motivation to pursue the study of quantum theory in the rest of the course.

Learning goals of the lecture:

(a) Understand the experimental results that led to the development of Quantum Theory.

(b) Understand that quantum theory is necessary to describe the structure and properties of electrons, atoms and molecules.

(c) Understand that both matter particles and light have a dual wave/particle character.

9.2   HC2: The quantum wave-function and Schroedinger equation

The Schroedinger equation, the quantum wave-function, the Born interpretation, mathematical tools of quantum mechanics, the free particle, Heisenberg's uncertainty principle.

Based on Atkins and de Paula, *Physical Chemistry*, 10th edition, Chapter 7.

In this lecture we present the mathematical framework of quantum theory, where the main entity is the *quantum wave-function*, and the dynamical equation that this wave-function must obey, the Schroedinger equation. We also introduce a number of mathematical tools which are required in the quantum formalism. We discuss Heisenberg's uncertainty principle, and show that it entails a fundamental limitation about the physical knowledge that we can have about quantum systems.

Learning goals of the lecture:

(a) Understand that the state of a quantum system is described by the quantum wave-function, which is a solution of the Schroedinger equation.

(b) Understand and apply the mathematical description of quantum physics, including hermitian operators, eigenvalue equations and orthogonality.

(c) Understand how experimental observables can be calculated from the wave-function, and perform these calculations in simple systems.

(d) Understand the Copenhague interpretation of the physical meaning of the wave-function.

(e) Understand and apply Heisenberg's uncertainty principle in different situations, in its two versions between position and velocity and between energy and time.

9.3   HC3: Quantum mechanics of simple systems

> Quantum mechanics of simple systems: the particle in a box, quantum tunneling, the quantum harmonic oscillator, particle in a box with finite potential barriers.
>
> Based on Atkins and de Paula, *Physical Chemistry*, 10th edition, Chapter 8.

In this lecture we discuss quantum mechanics applied to relatively simple systems such as the particle in a confining box and the quantum harmonic oscillator. We will study some remarkable phenomena that appear in these systems that do hot have an analog in classical mechanics, such as that the *the quantization of energies* and the *quantum tunneling*. For instance, we will show how a quantum particle can cross an energy barrier even if its energy is smaller than that of the barrier. You will also start to carry out simple calculations that will train you for the more difficult calculations in the following sections.

Note that this lecture assumes the knowledge of ordinary differential equations. If you are not familiar with them, please revise your previous courses in Mathematical Analyses.

> The *learning goals* of this lecture are:
>
> (a) Solving the Schroedinger equation for simple quantum systems.
>
> (b) Understanding that confinement of a quantum particle in space leads to the quantization of its energy levels, with an non-vanishing energy for the ground state.
>
> (c) Interpret the physical content of the wave-functions from the solutions of the Schroedinger equation.
>
> (d) Understanding and applying the mathematical technique of separation of variables.
>
> (e) Understanding and applying the phenomenon of quantum tunneling.

9.4   HC4: The Schroedinger equation for systems with rotational symmetry

> Molecular and Vibrational Spectroscopy
>
> Based on Atkins and de Paula, *Physical Chemistry* 10th edition, Chapter 9

In this lecture we continue with the applications of the Schroedinger equation for important physical systems, in this case in the presence of rotational symmetry such as a particle moving on a ring or on the surface of a sphere. We will also introduce the concept of intrinsic angular momentum of a particle, known as *spin*. Learning how to solve the Schroedinger equation in these systems will allow us then in the next lectures to compute the structure of electronic levels in atoms and molecules.

> The *learning goals* of this lecture are:
>
> - To be able to solve the Schroedinger equation for a rotating particle, specifically in the two-dimensional (particle on a ring) and three-dimensional (particle on a sphere) cases.
>
> - To understand the mechanism by means of which rotational symmetry leads to the quantization of of the physically allowed energy levels.
>
> - To interpret physically the solutions of Schroedinger equation for a rotating particle, in particular in terms of their probability distributions.
>
> - To become familiar with the concept of *spin* (intrinsic angular momentum) in quantum mechanics.

9.5   HC5: The hydrogen atom

Molecular and Vibrational Spectroscopy

Based on Atkins and de Paula, *Physical Chemistry* 10th edition, Chapter 10

In this lecture we will study in some detail the solutions of the Schroedinger equation applied to the hydrogen atom, and display the connection with the empirical assumptions of Bohr's atomic model. We will show how important features of the electronic structure of atoms can be already will modelled by this system, in particular the classification of electronic levels in terms of energy and angular momentum quantum numbers. A detailed understanding of the electronic structure of the hydrogen atom will allows us first to describe multi-electron atoms and then in subsequent lectures to describe the electronic structure of molecules.

The *learning goals* of this lecture are:

- To determine a suitable coordinate system to express the Schrdinger equation applied to the hydrogen atom in a physically transparent way.

- To learn how to solve the Schrdinger equation for the hydrogen atom by using the method of separation of variables.

- To be able to provide a physical interpretation of the radial and angular wave functions of the hydrogen atoms in terms of probability densities.

- The understand how these solutions lead to the electronic structure of the hydrogen atom in terms of electronic levels and shells, in particular taking into account the role of angular momentum.

9.6   HC6: Multi-electron atoms and orbital theory

Molecular and Vibrational Spectroscopy

Based on Atkins and de Paula, *Physical Chemistry* 10th edition, Chapter 10

Building on the experience with the hydrogen atoms acquired in the previous lecture, here we take a step forward and move to solving the Schroedinger equation for atoms characterized by more than one electron, the s-called multi-electron atoms. This will require introducing a number of important concepts that were absent in the description of the hydrogen atom such as the idea of shielding, the Pauli and Aufbau principles, and the ideas behind how to combine the spin states of two particles.

The *learning goals* of this lecture are:

- To learn how to derive solutions for the Schrdinger equation for multi-electron atoms by means of the orbital approach.

- Understand a number of important concepts in multi-electron atoms such as shielding, the Pauli principle, and the Aufbau-principle.

- To become familiar with the concept of spin combination, in particular with the ideas of *singlet* and *triplet* states for a pair of particles with spin.

9.7   HC7: Molecular structure

> Molecular and Vibrational Spectroscopy
>
> Based on Atkins and de Paula, *Physical Chemistry* 10th edition, Chapter 11

This is the first of three lectures dealing with molecular structure, that is, aiming to understand the allowed energy levels that electrons can occupy in molecules composed by two or more atoms, as compared to the electronic levels of individual atoms described in the previous two lectures. We will present in this context the valence bond theory, based on the overlapping of individual atomic orbitals. We will also discuss the BornOppenheimer (BO) approximation, namely the idea that the motion of the electrons within a molecule takes place at a much higher speed than that of the atomic nuclear and that thus is becomes effectively decoupled from the latter.

> The *learning goals* of this lecture are:
>
> - To understand and be able to apply the valence-bond theory to homonuclear diatomic molecules as well as to multi-atomic molecules composed by more than two atoms.
>
> - To become familiar with the concept of molecular orbital and to be able to represent it in terms of the underlying probability density.
>
> - To understand the Born-Oppenheimer approach and to be able to use it in different configurations.
>
> - To be able to graphically represent the concept of hybrid molecular orbital.

9.8   HC8: Molecular Orbital theory and hybridization

Molecular and Vibrational Spectroscopy

Based on Atkins and de Paula, *Physical Chemistry* 10th edition, Chapter 12

In this lecture we continue our study of the electronic structure of molecules by presenting the Molecular Orbital theory, a method that allows to determine the molecular electronic structure where electrons are not assigned to individual bonds between atoms, but are rather treated as moving under the influence of the nuclei in the whole molecule. This will also leads us to the important concept of hybridization, describing the rules that govern how electronic orbitals in individual atoms can merge among them to give rise of molecular orbitals.

The *learning goals* of this lecture are:

- To understand and be able to apply the molecular orbital theory, based on the method of linear combinations of atomic orbital, to simple diatomic molecules.

- To be able to predict whether a specific molecular configuration will lead to orbital bonding or instead to anti-bonding.

- To manage to to draw up a molecular orbital energy diagram for homonuclear diatomic molecules.

- To understand the basic symmetry properties of molecular orbitals, with special emphasis on the role of angular momentum.

9.9   HC9: Huckel theory

Molecular and Vibrational Spectroscopy

Based on Atkins and de Paula, *Physical Chemistry* 10th edition, Chapter 12

This lecture completes the part of the course describing molecular structure, and is focused on the formulation of the so-called Huckel theory. This is a method based on the linear combination of atomic and molecular orbitals (LCAO MO) which allows to determine the energy levels of π electrons in conjugated hydrocarbon systems and other related molecules. Using Huckel methods, it is possible to derive the energies of some of molecular levels in important cases such as the butadiene molecule.

The *learning goals* of this lecture are:

- To understand and be able to apply the variational principle to an heteronuclear diatomic molecule.

- To become familiar with the mathematics and physics behind the Huckel approach.

- To be able to produce the complete Huckel matrix for a generic, not too large, molecule.

9.10   HC10: Molecular and vibrational spectroscopy

Molecular and Vibrational Spectroscopy

Based on Atkins and de Paula, *Physical Chemistry* 10th edition, Chapter 12

HC10 is the first of the last three lectures of the course. In this final part, we will discuss the *interaction of molecules and nuclei with different types of electromagnetic radiation*. First of all, in HC10 we will discuss the general properties of *molecular spectroscopy and vibrational spectra*, where by *spectroscopy* we understand the study of the interaction between electromagnetic radiation and matter using different experimental techniques. Then in HC11 we will study electronic transitions in molecules. Finally, in HC12 we will illustrate the underpinnings of Nuclear Magnetic Resonance (MNR), highlighting how quantum physics is central to one of the most widely used methods of medical imaging.

The *learning goals* of this lecture are:

- Understanding and applying the basic properties of absorption and emission of electromagnetic radiation in molecules.

- Become familiar with the vibrational states and the corresponding transitions among them for di- and poly-atomic molecules.

- Understand that vibrational transitions lead the interactions with infrared light via Raman scattering, and learn how to exploit this knowledge for practical applications.

9.11   HC11: Molecular spectroscopy and electronic transitions

> Molecular Spectroscopy and Electronic Transitions
>
> Based on Atkins and de Paula, *Physical Chemistry* 10th edition, Chapter 13

In this lecture, we will study electronic transitions in *p-electron conjugate systems*, the Franck-Condon principle, the physics underlying the phenomena of *fluorescence* and *phosphorescence*, as well as the basic principles of operation of a *laser*. We will also present an application of these ideas in the medical context, namely the *photo-dynamic therapy* (PDT).

> The *learning goals* of this lecture are:
>
> (a) Understanding and applying π-π^* electronic transitions in molecules.
>
> (b) Understanding which electronic transitions can take place for either absorption or emission of a photon while the atomic nuclei are at rest (the Franck-Condon principle), including the mathematical description and implications of absorption and emission spectra.
>
> (c) Understanding and applying the principles of fluorescence and phosphorescence.
>
> (d) Understanding the basic principles that underlie the operation of a laser, such as the concept of population inversion.

9.12   HC12: Magnetic Nuclear Resonance

Magnetic Nuclear Resonance

Based on Atkins and de Paula, *Physical Chemistry* 10th edition, Chapter 14

In this final lecture of the course, we will explore the important topic of Magnetic Nuclear Resonance and show it is the basis for one of the most important applications of quantum theory in medical therapy, namely *Magnetic Resonance Imaging*.

The *learning goals* of this lecture are:

(a) Understand that the atomic nucleus has a magnetic moment, and that upon interaction with a magnetic field its energy levels split for different values of z component of the nuclear spin.

(b) Understand and be able to interpret Nuclear Magnetic Resonance (NMR) spectra.

(c) Understand how pulse techniques can be employed in order to measure NMR spectra.

(d) Become familiar with the basic principles of Magnetic Resonance Imaging (MRI).

van Quantum tot Molecuul

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Course Assessment Plan

current version: October 19, 2017

Staff Developer: Dr Anja Swennen

Tutor: Prof Piet Mulders

Table of Contents

1   General context and introduction

In this document I present the detailed assessment that I prepared in the context of the redesign of the *"van Quantum tot Molecuul"* ("from quantum mechanics to molecules") course, which is part of the Bachelor in Medical Natural Sciences (*Medische Natuurwetenschappen*, MNW) offered by the VU.

Specifically, I discuss in this document the following issues related to the course assessment:

- How is the course assessed, both formative and summative?

- At what moments will assessment takes place? And by what type of test?

- Are all course objectives assessed? How can I show that the test fits the course objectives (validity)?

- How is reliability assured? How I you avoid arbitrariness?

- How do I ensure that the organization, development and implementation of the assessment is transparent for the students (transparency), and manageable for the teacher (usability)?

2   Course assessment: formative and summative

When discussing the various methods to assess a course, we need to make in important distinction between *formative assessment* and *summative assessment*. The definition of these two concepts is the following:

- *Formative assessment* aims to monitor student learning to provide ongoing feedback that can be used by instructors to improve their teaching and by students to improve their learning. Specifically, the goal of this type of assessment is to help students identify their strengths and weaknesses and target areas that need work, as well as to help instructors to recognize where students are struggling and address problems immediately. Most formative assessments are part the so called *low stakes* type, which means that they contribute little or none to the final course mark.

  Examples for formative assessment include drawing a concept map in class at the end of a lecture to demonstrate that they have grasped the various topics that have been discussed, or providing a first draft of an out-of-class assignment to collect initial feedback from the instructors.

- *Summative assessment* has instead the goal of evaluating the student learning at the end of an instructional unit. This is done by comparing the learning of the student with some predefined standard or benchmark. As opposed to formative assessments, summative assessments are often of the *high stakes* type, meaning that they carry a significant weight in the final grade of the course.

  Examples of this type of assessment include partial and final exams, out-of-class assignments, laboratory reports, or field-trip reports. The information from summative assessments is crucial in order to help both students and faculty to optimize their efforts in subsequent courses as well as in future installments of the same course.

In this context, the assessment of the *"van Quantum tot Molecuul"* course will be performed as follows. Concerning the *summative assessment of the course*, I will implement the following strategy:

- The first part of the course *summative assessment* will be composed by an *intermediate examination* towards the end of the first half of the course (*tussentoets*), followed by a *final test* at the end of the course, once all the lectures and tutorial sessions have been carried out (*volledig eindtentamen*). In the partial exam, the material that will be covered includes everything from the start to the course to the topics covered in HC6, while the final exam will cover all the course topics.

- Whether or not an student needs to carry out both Parts I and II of the final exam depends on the marks that she obtained during the partial exam (*tussentoets*). Specifically, if the grade obtained in the intermediate exam was insufficient, the complete final exam needs to be performed (Parts I+II). On the other hand, if the grade obtained in the exam is a pass or higher, there is the option to either skipping or attempting Part I in the final exam. In the latter case, the best of the two marks will be the one that counts for the course evaluation.

- The mark obtained in these two exams weights **75%** of the total course mark. In the appendix of this document I provide an explicit example of a course test that I prepared, including the corresponding solutions and the criteria that should be used to mark the various questions.

- Both during the partial and the final exam, the use of any external material such as textbook of formulae lists is not allowed. Likewise, the use of scientific programmable calculators us not allowed: the students are allowed to bring only a simple calculator without memory for mathematical expressions. Together with the exam, a list of potentially useful physical equations, mathematical relations and physical constants will be provided to the students.

- The second part of the course's *summative assessment* is based on *tutorial sessions* supervised by the Teaching Assistants (TAs). In total there are 9 of such tutorial sessions, and attendance to the tutorials is compulsory (else examination will not be allowed).

- During these tutorial sessions (which last 2 hours, same as the theory lectures), the students are given a number of *exercises to carry out in the class*, covering the same topics as those discussed in the previous theory lectures. The TAs will assist the students in their problem-solving activity, but are not supposed to give *i.e.* the full solution of the problems in the blackboard: the main motivation of such sessions is that the students *learn by themselves how to solve the problems*. Note that the TAs will carry with them the solutions of all the problems, so they can indicate whether someone has obtained the correct or the wrong answer to some specific exercise.

- In this respect, in order to take the most profit of these tutorial sessions, it is very important that the students prepare in advance the tutorial work for each session. To this aim, we will propose that the students *self-organise themselves in groups of three or four* students to prepare beforehand the tutorial work for each session.

- At the beginning of each tutorial session, the TAs will indicate *two specific problems* (out the entire list that had been indicated in **Canvas** beforehand), which the students will need to carry out and then hand in to the TAs. The average mark of all the problems that the students have handed in during the nine tutorial sessions will contribute to the **25%** of the total course mark.

Concerning the *formative assessment* part of the course, it consists on the following activities:

- First of all, the *problems done during the tutorial sessions* under the supervisions of the TAs. While only two of these problems counts towards the final grade, working on the other problems and using the feedback from the TAs will help the students to synthesize and apply the basic concepts that they have learned in the theory sessions.

- In addition, it is possible to *submit specific questions by email or to post them in* **Canvas** *about the exercises to the TAs* at any point during the course, including about problems covered in previous tutorial sessions. In this respect, the *formative assessment* of the course extends beyond the classroom activities.

- Specifically, the idea is that **Canvas** provides an *on-line forum* where the students can discuss both among them and with the TAs about the best way to solve specific problems with no time limitations. This also helps with the students that have missed some previous tutorial session, since in **Canvas** their will have an archived backlog of all the discussions associated to an specific problem. This forum will be monitored by the TAs of the course, to ensure that only issues relevant to the course are discussed, and to avoid anti-social behaviour.

- Another integral component of the *formative assessment* activities of the course are the *short in-class activities* that will be carried out during each of the theory lectures. As illustrated in the two *Lesson Plans* that I have prepared (see attached document), during the lecture the students will be engaged in a number short in-class activities. For example, in the specific case of the Lesson Plan for HC2, these activities will be the following:

  - I will check with the students how familiar are with the mathematical concepts of eigenvalue equations. I will do this by presenting them with four different eigenvalues equation and asking them using *Mentimeter* which ones they had worked with before.

  - They will have to do a *quick exercise* (5 min max) in groups of two, namely solving an eigenvalue equation and determining the corresponding eigenvalues.

  - Working in groups of three, the students have to apply the Heisenberg principle to determine the uncertainty on the position of a i) a car, ii) an atom, and iii) an electron. I will provide all the numerical values of the input parameters, and then the students need to compute the results and to provide the corresponding physical interpretation.

- While these in-class activities are not part of the summative assessment of the course (this is carried out during the tutorial sessions) but rather of the *formative assessment*, they will provide very useful feedback to the instructors to monitor the progress of the students and to assess in which topics they are still somewhat weak.

3 Revised assessment plan

Here I present a revised assessment plan for the *van Quantum tot Molecuul course*. Each row indicates the main topics that should be covered during the course, and that summarize the *associated learning objectives*. Then in the various columns I indicate at which point of the course the students:

- Should know and understand each specific topic

- How exactly they should be able to apply and analyze it,

- How each topic will be evaluated

- Possible creative applications of selected topics.

van Quantum tot Molecuul
Assessment plan

Topic	Know	Understand	Apply+Analyze	Evaluate	Create
Schroedinger equation for simple quantum systems	*Week 2*	*Week 3*	*Free particle Particle in a box Harmonic oscillator*	*Partial exam*	
Electronic transitions in the hydrogen atoms	*Week 4*	*Week 5*	*Electronic transitions Calculation of electronic shell structure*	*Partial exam*	
Electronic transitions in the multi-electron atoms	*Week 6*	*Week 7*	*Modified electronic transitions as compared to hydrogen atoms*	*Partial exam*	*Small assignment project: understand experimental data on molecular electronic transitions*
Molecular spectroscopy	*Week 8*	*Week 9*	*Identifying molecules from their radiation pattern*	*Partial+final exam*	
Vibrational spectroscopy	*Week 9*	*Week 10*	*Identifying molecules from their vibrational radiation patters*	*Partial+final exam*	
Magnetic nuclear resonance	*Week 10*	*Week 11*	*Describe mathematically the function of an MNR scanner*	*Partial+final exam*	*Small assignment project: applications of quantum theory in medical sciences*

Figure 3.1: Assessment plan of the course.

4   Achieving the course objectives

I now move to discuss how I will assess that the course objectives have been appropriately attained by the students. In doing this, I will also show that the assessment strategies that I propose are really suited to gauge the realization of the course objectives (validity).

Validity is a very important concept when considering assessment design. For instance, most course assessments include some form of exam or test. In this respect, it is crucial to make sure that the score that a given student achieves in a test is a reasonably *good proxy of his/her actual performance*, else it becomes impossible to meaningfully interpret the tests results. In this context, by *assessment validity* one means that the design of a given assessment strategy should be such that its results, for example of a test, reflect the original purpose of the assessment, such as for example attaining the learning goals of the course. From the formal point of view, validity is defined as the *process of constructing and evaluating arguments for and against the identified interpretation of test scores and their relevance to the proposed use.*[1].

In the context of the present revised assessment plan, the *validity of the assessment* aiming to determine in a reliable way how the course objectives are achieved by the students (in other words, their *validity*) is demonstrated by the following considerations:

- The questions that compose both the partial and the final exams have been carefully chosen in way that they math the *course objectives in a one-to-one basis*. In other words, the questions that compose the final exams are representative of the overall course objectives, ensuring that a student that is able to get a *pass* in the exam has satisfactory attained the majority of the course objectives.

- To illustrate this point, let me take two of the questions of the example test that is provided in the appendix of this document. The first question that I have chosen is the following:

  - **Q.** *Discuss briefly the Frank-Condon effect in vibronic transitions. Assume that the ground vibrational state of a molecule is given by the particle-in-a-box wave-function, with*

  $$\psi_0(x) = (2/L)^{1/2} \sin(\pi x/L) \,, \tag{4.1}$$

  for $0 \leq x \leq L$, and 0 elsewhere. By evaluating the overlap between wave functions, compute the Frank-Condon factor for a transition to a excited vibrational state described by the wave-function

  $$\psi_1(x) = (2/L)^{1/2} \sin(\pi(x - L/2)/L) \,, \tag{4.2}$$

  for $L/2 \leq x \leq 3L/2$, and zero elsewhere. Sketch the two wave functions and schematically illustrate the direction of the vibronic transition.

  This question corresponds directly to the following course objectives (as indicated in the *revised course guide*):

  - *Understand how experimental observables can be calculated from the quantum wave-function as a solution of the Schrödinger equation with different symmetries and boundary conditions, and perform these calculations in simple systems.*

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[1] http://ctl.yale.edu/AssessmentDesignValidity

– *To become familiar with the concept of molecular orbital, and to be able to represent it in terms of the underlying probability density. This goal also involves being able to combine electric orbitals from individual atoms into joint molecular orbitals.*

The reason is that this problem requires both a good understanding of the basic principles of quantum theory as well as being able to apply them in the context of electronic transitions between molecular electronic levels. Therefore, a students that answers this question correctly has clearly demonstrated that at least this two course objectives have been satisfactory attained.

The second example question from the course exam that I wanted to use to illustrate the direct connection between the course's *summative assessment* and the validity of achieving the course objectives is the following:

– *Discuss qualitatively the concept of resonant (Larmor) frequency of an atomic nucleus embedded in a external magnetic field. What is the resonance frequency of a ^{19}Fe nucleus in a magnetic field of 17.1 T? This atomic nucleus has spin 1/2 an nuclear g-factor of $g = 5.2567$*

This question corresponds directly to the following course objective (as indicated in the *revised course guide*):

– *Become familiar with the basic principles of Magnetic Resonance Imaging, and understand how the spin of atomic nuclei represents one of the most helpful ingredients of modern medical imaging.*

A student that is able to satisfactorily answer this question has demonstrated that she has a good understanding of the Magnetic Resonance Imaging, and knows how to apply calculations in quantum theory to understand the properties of the spin of atomic nuclei. So also in this case, a student that answers correctly this question demonstrates that she/he has a good understanding of this specific course learning objective.

Taking into account all the questions in the exam, the totality of course learning objectives are covered, thanks to this *direct correspondence* between learning objectives and specific exam questions.

• The same basic principle holds for compulsory problems to be carried out during the tutorial sessions, which add up to **25%** of the total course mark. That is, the specific choice of exercises for the problem-solving sessions is made in order to ensure a *direct correspondence with the course learning objectives*. This means that a student that performs on average well in all these problems, will also on average have attained a satisfactory understanding of the course learning objectives.

For these reasons, I consider that the assessment plan that I propose has a well-defined *validity*, that is, it is suitable to monitor the original motivation of the assessment strategy, in this case to verify that the students have satisfactorily achieved the course objectives.

5   Assessment reliability

Next I move to discuss the important topic of how is *reliability* assured, and of how I avoid *arbitrariness* in assessing the students.

Before doing that, let me first give the formal definition of *reliability*.[2] This concept refers to the extent to which *assessments are consistent*, that is, that one should strive to have *reliable, consistent instruments to measure student achievement.* This means specifically that results of assessment tools such as the marking of an exam or of an assignment should be the same, whether a student takes the assessment in the morning or afternoon; one day or the next, or whether the assignment is handed in on the first day of the term or the last day before the deadline.

Another measure of reliability is known as the *internal consistency of the items.* For instance, assume that one has a test where four questions are related to the specific knowledge of the student concerning a specific course learning objective. If the test questions are consistent among them, and they all refer to the same course objective, one expects that on average if a students does well on one question he/she will also perform well in the rest of the questions of the group, and vice-versa. If this does not happen, the test is considered as *internally inconsistent* and therefore this specific choice of assessment tool is considered as unreliable.

In order to guarantee both the *reliability* and the *internal consistency* of the assessment methods that have been discussed above, the following factors have been taken into account:

- The partial and final exams will be *marked independently by two instructors.* We will them compare the marks that each student has obtained in each question, and where the marks different by more than a given statistical threshold (which is usually taken to be **20%** of the total weight of that specific question) we will look together at this question and agree together which is the fairest mark.

- Moreover, we will keep a detailed record of on how many occasions the two independent markings lead to different results. If the fraction of questions where there is no consensus in the mark is too large, that would imply that the marking instructions are ambiguous, and we will strive to produce future exam questions without that limitation.

  This is specially important for the partial exam: there we can gather important information to ensure that the final test is *fully reliable.* In addition, one should aim to have a downward trend of this year after year, in a way that exams scores become as reliable as possible.

- The *internal consistency* of the test results will be validated by means of a detailed statistical analysis of the test scores. Specifically, we will cluster the results of the questions by relevance to the various learning objectives (see the discussion in the previous section) and then construct the underlying probability distribution using the *Kernel Density Estimation* method[3], which is a non-parametric algorithm to estimate the probability density function of a random variable using a finite sample of results (in this case the test scores).

  The use of this statistical analysis will allow us to identify possible issues with the *internal consistency* of the tests results. This can be done in various ways. For example, the probability distribution of different questions that are related to the same course learning objective should be *highly correlated* among them, else the chosen set of exam questions is internally inconsistent.

  As an important byproduct of the statistical analyses of the test results, it will also be possible to determine how *fair* the exams questions have been. For instance, if the *mean/median of the results* is

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[2] Definition taken from https://fcit.usf.edu/assessment/basic/basicc.html
[3] https://en.wikipedia.org/wiki/Kernel_density_estimation

significantly below the *pass mark* (within say the 68% confidence level interval) this would mean that the exams questions were too difficult for the average students, and that the distribution of marks should be rescaled to match with the *ideal* distribution, in which the pass mark falls within the 68% confidence level internal of the exam mark distributions.

- The same considerations apply to the marking of the exercises carried out during the tutorial sessions. Each set of problems will be evaluated for two of the course's TAs, and if the discrepancy between the two marks is above the threshold, the third TA will make the same specific set of problems again. The final mark will be then constructed by *taking the average of the marks provided by each TA*.

These measures ensure that the proposed course assessment will be as *reliable* and *internally consistent* as possible. In particular, the two key measures are the marking of both the exams and of the in-class problems by more than one assessor, and a detailed statistical analysis of the distribution of test scores in order to identify and correct any possible lack of reliability, internal inconsistency, or inadequate overall difficulty of the test questions.

6   Transparency and usability

In the final part of this revised assessment plan, I discuss how do I ensure that the organization, development and implementation of the assessment is transparent for the students (*transparency*), and manageable for the teacher (*usability*).

As in the previous sections, let us first start with a brief reminder of the formal definitions of these two important concepts. To begin with, one understands that an assessment is *transparent* when all the parties involved, from instructors to students, teaching assistants, and assessors, fully understand in advance what is required in the assessment how the candidates' work or performance will be graded and marks awarded. For example, in the case of a written test, we can consider it as *transparent* if everyone involved knows in advance the weight that each question will carry on the overall test score, and even more, how the mark of such question will be assigned in the case of a partial and/or incomplete answer. Among the various benefits of *transparency in assessment* is that students understand how and why their learning of the course content is being assessed in that specific way, giving them reassurance and motivating that their work will be assessed in a fair way.

In a related formulation, *transparency* is also related to the how clear the assessment expectations are for students.[4]. To *quantify is a specific assessment method is transparent*, some of the relevant questions that need to be taken into account are the following:

- Did students understand what was required of them to succeed in the task set for them?

- Did students know in advance what it is they are expected to do, and how the various parts of their assignments will be marked?

- Do students understand against which baseline they will be assessed? That is, is there a clear score scale that separates a satisfactory from an unsatisfactory performance in the assessment?

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[4]https://app.griffith.edu.au/assessment-matters/docs/design-assessment/principles/transparent

- Do instructors provide model examples so that the students know the level of performance expected? This could be for example solved exams of previous years, or class assignments and reports of previous years that have achieved the highest possible marks.

Concerning the other concept, the formal definition of *assessment usability* is that the organization, development and implementation of the assessment can be *satisfactorily managed by the instructors*. In other words, an excellent assessment plan in theory might not be *usable* in practice if for example it requires an unreasonably large workload or it not possible to implement in practice due to technical considerations. An example of the latter would be when a specific assessment task requires that all students bring their laptops into class, but a fraction of the students do not have personal laptops and therefore this specific assessment strategy cannot be used.

When designing the present revised course assessment, I have taken care to ensure that the specific assessment strategy that will be adopted is both *transparent* and *usable* as demonstrated by the following considerations:

- In the study guide we indicate carefully beforehand the *relative weight* that each of the assessment components has on the final grade. They know that the exams count **75%** of the total grade while the in-class exercises count **25%**. And they are aware that the two specific exercises that will be marked in each tutorial session are chosen within the list of pre-defined exercises, so they have ample time to revise and to prepare for them before the tutorial.

- In addition, they know which conditions in detail they should fulfill in order to pass the partial exam and be able to carry out only the second half of the second and final exams. Thanks to this *transparency in the exam conditions*, the students can take informed choices of what would be their best strategy concerning taking the full final exam, or only the questions corresponding to the second half of the course.

- The students can have access in **Canvas** to several examples of past exams (both for the total and for the partial) together with the corresponding detailed solutions and scores marks. This way, the students know how their own exams will be evaluated, since they have the references of previous exams, and there is no ambiguity about how the marking is performed.

- After both the partial and final exams, the students are provided with the corresponding solutions and therefore they can verify their performance with respect to the example solution. In case they are unhappy with the marking of some specific questions, they can discuss it with the instructors, though in the past this has happened only a very reduced number of times.

- The workload involved in all the assessment tasks is fully manageable both by the instructors, the teaching assistants, and the course assessors. Marking the exams take in total around 2 days of full time work, with one additional days to prepare the questions with the corresponding model solution sheet. This is included in the total time that the instructors should spend in their overall teaching activities.

- Consistently with the above statement, the teaching assistants need to spend at most 2 hours after every tutorial sessions marking their problems, for a total of 18 hours during the full duration of the course. This amount is well within the total time that they are expected to spend in teaching activities.

A   Example of final exam

In this appendix I present a representative test (specifically the one we used for the final exam earlier this year) of the *"Van quantum tot Molecuul"* course.

A.1   Introduction and grading instructions

In the following I provide an explicit example of the final exam that would be used to assess whether of not the students have properly achieved the *learning objectives at the end of the course.* The exam is divided into four questions, each of them contributing equally to the total mark. Therefore, each of the four questions listed here contributes to **25%** of the total exam mark, which in turn corresponds to **75%** of the total course mark (with the rest of the course mark being provided by the in-class exercises, as indicated above). To get the full mark in each question, the students needed to obtain the correct numerical answer, and moreover to justify in detail the various steps carried out in order to solve the problem.

As mentioned above, the instructors are provided with the explicit solution of each problem, also included here for completeness.

Concerning the marking instructions, they are the following:

- To achieve the *full mark* of an specific question, the students should both get correct the *numerical solution* of the question and the detailed *physical justification* of the specific approach that they have used.

- If they provide the correct numerical result of the exercise, but miss the physical justification and/or interpretation of the result, they get only *half the maximum mark.*

- Conversely, if they provide the right physical interpretation or motivation of an specific question, and set up the correct set of equations, but fail to get the correct numerical answer, they get *half the maximum mark.*

- If the students fail to give both the correct numerical result and the correct physical justification, they *do not get any points* for this specific question.

In case there could be ambiguities in some specific questions (for example those without numerical answers) the example model sheet will provide explicit instructions in such case.

A.2   Exam questions

- **Q1**. *Calculate the percentage difference in the fundamental vibrational wavenumber of $^{23}Na^{35}Cl$ and $^{23}Na^{37}Cl$ assuming that the spring constants of these two molecules are the same.*

  A1. The frequency of the vibrational modes of a diatomic molecule is given by

  $$\omega = \sqrt{\frac{k_f}{m_{\text{eff}}}}\,, \tag{A.1}$$

  where k_f is the spring constant and m_{eff} the effective mass. Their fractional difference will be therefore given by the ratio of effective masses,

  $$\frac{\omega' - \omega}{\omega} = \sqrt{\frac{m_{\text{eff}}}{m'_{\text{eff}}}} - 1 = -0.0107\,. \tag{A.2}$$

  So due to the difference in atomic masses, the fundamental vibrational wave-numbers of these two molecules will differ by 1.1%.

  Note that the effective mass of a two-body system is defined as:

  $$m_{\text{eff}} = \frac{m_1 m_2}{m_1 + m_2} \tag{A.3}$$

  Therefore we have that for this specific combination of molecules:

  $$\frac{\omega' - \omega}{\omega} = \sqrt{\frac{m_{\text{eff}}}{m'_{\text{eff}}}} - 1 = \left(\frac{m_{23Na} m_{35Cl}}{m_{23Na} + m_{35Cl}} \times \frac{m_{23Na} + m_{37Cl}}{m_{23Na} m_{37Cl}} \right)^{1/2} - 1 \tag{A.4}$$

- **Q2.** *Discuss briefly the Frank-Condon effect in vibronic transitions.*

  Assume that the ground vibrational state of a molecule is given by the particle-in-a-box wave-function, with

  $$\psi_0(x) = (2/L)^{1/2} \sin(\pi x/L) \,, \tag{A.5}$$

  for $0 \leq x \leq L$, and 0 elsewhere. By evaluating the overlap between wave functions, compute the Frank-Condon factor for a transition to a excited vibrational state described by the wave-function

  $$\psi_1(x) = (2/L)^{1/2} \sin(\pi(x - L/2)/L) \,, \tag{A.6}$$

  for $L/2 \leq x \leq 3L/2$, and zero elsewhere. Sketch the two wave functions and schematically illustrate the direction of the vibronic transition.

  You might find the following indefinite integral useful:

  $$\int \sin(ax) \sin(ax + b) = \frac{x}{2} \cos(b) - \frac{\sin(2ax + b)}{4a} \,. \tag{A.7}$$

A2. A vibronic transition is a molecular transition in which both the electronic and vibrational states of the molecule are simultaneously modified. The Frank-Condon principle states that in the vibronic transition with the highest rate is the one for which the electronic state of the molecules changes with the smallest change in the relative separation of the atoms within the molecule. When plotted in the $V(r)$ plane, the Frank-Condon principle states that vibronic transitions are more likely to be vertical.

The overlap between the two wave functions is given by

$$S(v,0) = \langle v|0 \rangle = \frac{2}{L} \int_{L/2}^{L} \sin(\pi x/L) \sin(\pi(x - L/2)/L) \,, \tag{A.8}$$

and now if we define $a = \pi/L$ and $b = -\pi/2$ we can write the above integral as

$$S(v,0) = \frac{2}{L} \int_{L/4}^{L} \sin(ax) \sin(ax + b) = \frac{2}{L} \left[\frac{x}{2} \cos(b) - \frac{\sin(2ax + b)}{4a} \right]_{L/2}^{L} \tag{A.9}$$

where have have used the integral given in the problem question. This integral can be simplified to give:

$$S(v,0) = -\frac{1}{2\pi} \left[\sin(3\pi/2) - \sin(\pi/2) \right] = \frac{1}{\pi} \,, \tag{A.10}$$

and therefore the Franck-Condon factor for this vibrational transition is

$$|S(v,0)|^2 = \frac{1}{\pi^2} \,. \tag{A.11}$$

The physical interpretation is that the rate of a specific vibronic transition will be proportional to its Franck-Condon factor.

- **Q3.** *Describe the mechanisms of fluorescence and of phosphorescence. Explain why one of these two mechanism is much slower than the other. In the fluorescence mechanism, is the emission spectra an exact mirror image of the absorption spectra? You might want to complement your explanation by drawing a Jabloskly diagram.*

A3. *Phosphorescence* is a much slower process, taking place in an interval of *microseconds or more*, than *fluorescence*, taking place within a time interval of *nanoseconds* or less. The reason why phosphorescence is much is much slower is because it involves an electronic transition where the molecule goes from a *singlet* excited state to a *triplet* excited state via the so-called inter-system crossing, as illustrated in Fig. A.1 The resulting triplet states are long-lived, since a transition to the ground state is forbidden by the selection rules (Pauli exclusion principle).

In fluorescence, the emission spectra is red-shifted (reduction in photon energy) as compared to the absorption spectra due to the existence of non-radiative vibrational transitions which decrease the energy of the molecule without involving photon emission.
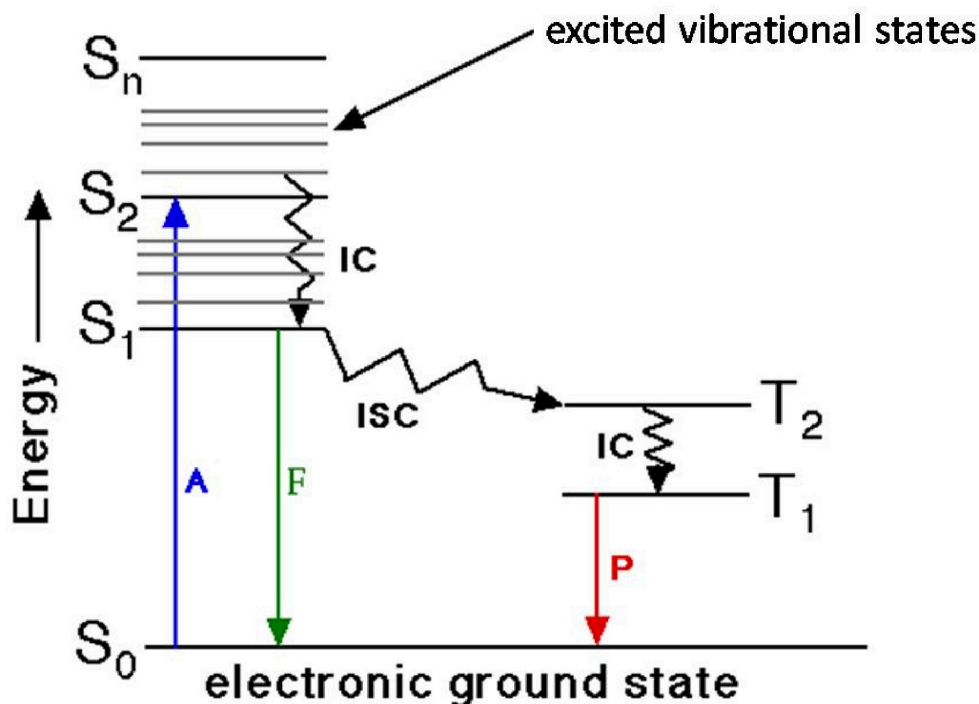
Figure A.1: Schematic representation of the fluorescence and phosphorescence phenomena by means of the *Jablonski diagram*. In this diagram, A indicates the absorption of a photon, F and P represent the fluorescence and phosphorescence transitions respectively, S and T denote singlet and triplet states, and finally IC and ISC label the internal conversion and the inter-system crossing respectively.

- **Q4.** *Discuss qualitatively the concept of resonant (Larmor) frequency of an atomic nucleus embedded in a external magnetic field.*

  What is the resonance frequency of a ^{19}Fe nucleus in a magnetic field of 17.1 T? This atomic nucleus has spin 1/2 an nuclear g-factor of $g = 5.2567$

  A4. In general, atomic nuclei have non-zero spin. Therefore, in the presence of an external magnetic fields, different spin states will have associated different energy values. The Larmor frequency is the frequency of electromagnetic radiation that is able to include transition between the two spin levels of an atomic nucleus.

  For the ^{19}Fe nucleus, the Larmor resonance frequency is given by

  $$\nu_L = \frac{\gamma_N B_0}{2\pi}\,, \quad \gamma_N = \frac{g_I \mu_N}{\hbar}\,, \tag{A.12}$$

  and now using that the nuclear magneton is $\mu_N = 5.0508 \times 10^{-27}\ \mathrm{J\,T^{-1}}$, we find that for this atomic nucleus the resonance magnetic frequency is

  $$\nu_L = 6.85 \times 10^8\,\mathrm{Hz} = 685\,\mathrm{MHz}\,. \tag{A.13}$$

  which correspond to the range of radio waves in the electromagnetic spectrum.

van Quantum tot Molecuul

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Lesson Planning

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1 General context

In this document I present two detailed *lesson plans* that I prepared in the context of the *"van Quantum tot Molecuul"* ("from quantum mechanics to molecules") course, which is part of the Bachelor in Medical Natural Sciences (*Medische Natuurwetenschappen*, MNW) offered by the VU.

For each of the two lesson plans, I describe:

- The explicit learning objectives that should be attained in that lesson.

- The preparation that the students should carry out before the lesson.

- The actual lecture contents, including graphic content when relevant.

- The in-class activities.

- The summary and overview of the lecture.

- A time planning explaining how the total lecture time will be divided into its various components.

- How I will assess the work of the students and which feedback will I obtain from them.

Each of the lessons is schedule to last for about two hours, with a 10 minute pause in the middle. So when preparing the lecture I have assumed that the total available time is 50 min + 50 min.

2   Lesson Plan I

HC2: The quantum wave-function and Schroedinger equation

2.1   Overview of the lecture

In this lecture I will present the mathematical framework of quantum theory, where the main entity is the *quantum wave-function*, and the dynamical equation that this wave-function must obey, the Schroedinger equation. I will also introduce a number of mathematical tools which are required in the quantum formalism. I will discuss as well Heisenberg's uncertainty principle, and show that it entails a fundamental limitation about the physical knowledge that we can have about quantum systems.

Learning goals of the lecture:

(a) Understand that the state of a quantum system is described by the quantum wave-function, which is a solution of the Schroedinger equation.

(b) Understand and apply the mathematical description of quantum physics, including hermitian operators, eigenvalue equations and orthogonality.

(c) Realize how experimental observables can be calculated from the wave-function, and perform these calculations in simple systems.

(d) Become familiar with the Copenhague interpretation of the physical meaning of the wave-function.

(e) Apply Heisenberg's uncertainty principle in different situations, in its two versions between position and velocity and between energy and time.

2.2   Resources and preparation

The contents of this lecture will be based on the course textbook, Atkins and de Paula, *Physical Chemistry*, 10th edition, Chapter 7. They should read the relevant sections of this chapter before the lecture. In addition, the lecture notes (handouts) will also be made available before the lecture on Canvas, and the students will be encouraged to take a look at them beforehand.

2.3   Topics to be covered during the lecture

In the following I indicate that various topics that will be covered during the lecture. After that, I indicate in a table below the amount of time that should be devoted to each topic, as well as to the additional in-class activities that will be carried out during the lecture. Here I also indicate the visual material that will be shown during the lecture, in particular those graphs that are used to illustrate the consequences of the theory concepts that have been introduced.

The quantum wave-function and Schroedinger's equation.   In quantum theory, the mathematical entity which is used to describe the motion of particles is known as the *quantum wave-function* Ψ. The *complete physical properties of any quantum system* are uniquely determined once its wave-function Ψ is specified. The wave-function depends on the spatial and time coordinates of the N particles that constitute the quantum system,

$$\Psi = \Psi\left(x_1, y_1, z_1, t_1, \ldots, x_N, y_N, z_N, t_N\right) . \tag{2.1}$$

The wave-function Ψ for a quantum system composed by a single particle satisfies the *Schroedinger equation*, which in one dimension x reads

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} + V(x)\Psi(x) = E\Psi(x) \tag{2.2}$$

The solution of this equation, $|\Psi(x)|^2$, represents the *probability density* in the coordinate x for this particle. Regions in x where $|\Psi(x)|^2$ is higher correspond to those regions where the particle has a higher likelihood to be found when a measurement is performed. This interpretation is known as the *Born interpretation of the wave-function*, and is illustrated in Fig. 2.1.

The Schroedinger equation for a free particle.   The simplest case that we can study with the Schroedinger equation is that of the motion of a *free particle*, that is, a particle which is not subjected to any form of potential, and thus has $V(x) = 0$. In this case the Schroedinger equation Eq. (2.2) takes the following particular simple form:

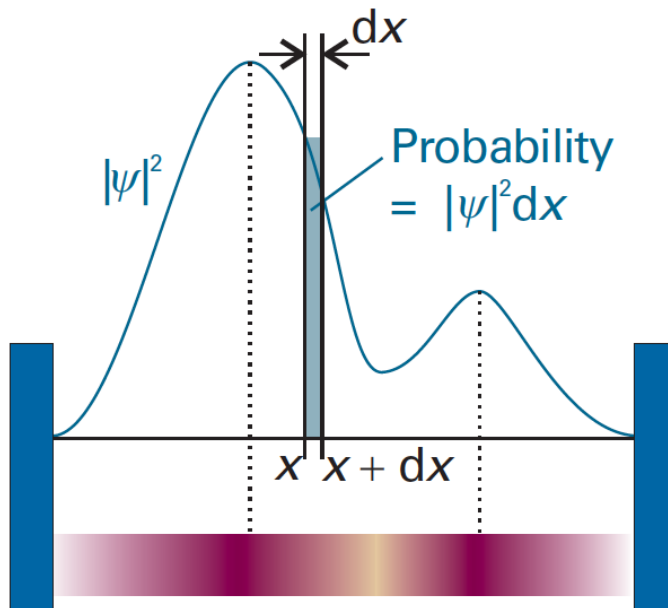$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} = E\Psi(x) \tag{2.3}$$

Figure 2.1: The physical interpretation of the quantum wave-function $\Psi(x)$ is that its square $|\Psi(x)|^2$ is the *probability density* associated to measuring the particle in a position x in space. Therefore, the *probability* to find the particle at position x in the range dx will be given by $|\Psi(x)|^2 dx$.

which is a second-order ordinary differential equation (ODE) that admits a solution in terms of a sum of exponentials (also known as *plane-wave* solutions):

$$\Psi(x) = Ae^{ikx} + Be^{-ikx}, \tag{2.4}$$

where A and B are the *integration constants*, to be fixed by the initial conditions of the system.

Eigenvalue equations in quantum theory.   Mathematically, the tools that we will use to compute the expected outcome of a measurement of a quantum system are known as *operators*, which can be expressed in the language of *eigenfunctions* and *eigenvectors*. Formally, an *operator* is a way to represent the action of a specific mathematical function onto the wave-function Ψ. For instance, Schroedinger's equation Eq. (2.2) can be expressed in operator form as follows

$$\hat{H}\Psi(x) = E\Psi(x), \tag{2.5}$$

where the ^ symbol indicates an operator, in this case the *Hamiltonian operator*, defined as

$$\hat{H} \equiv -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x). \tag{2.6}$$

An equation of the form of Eq. (2.5) is known as an *eigenvalue equation*, and are ubiquitous in many fields of physics from quantum theory to electromagnetism and thermodynamics.

Operators and physical observables in quantum theory. In quantum theory, the eigenvalues of specific operators, such as the Hamiltonian $\hat{H}$, correspond to *observables* of the system, in this case the total energy. Indeed, *each observable* of a quantum system, such as position, momentum, or angular momentum of the constituent particles, will have *associated an operator* that, when acting on the wave-function, will return the corresponding physical property as the eigenvalue. In quantum mechanics, any *observable property* Ω of the quantum system will be represented by an operator $\hat{\Omega}$ built up from the *position* and *momentum* operators, defined respectively as

$$\hat{x} \equiv x \,, \tag{2.7}$$

$$\hat{p}_x \equiv \frac{\hbar}{i} \frac{d}{dx} \,. \tag{2.8}$$

Generic operators, such as the energy operator $\hat{H}$, can be constructed by means of a suitable combination of the $\hat{x}$ and $\hat{p}_x$ operators.

Hermitian operators and orthogonality. In quantum mechanics, observable properties of a system have associated operators, whose eigenvalues correspond to the values than these observables can take when the measurement is performed. Only operators which are *Hermitian* are physically allowed. An Hermitian operator $\hat{\Omega}$ is such that, given two arbitrary wave-functions Ψ_i and Ψ_j, it satisfies the following property:

$$\int dx \Psi_i^* \hat{\Omega} \Psi_j = \left(\int dx \Psi_i^* \hat{\Omega} \Psi_j \right)^\dagger \,. \tag{2.9}$$

It is easy to check that both the momentum and position operators $\hat{x}$ and $\hat{p}$ are Hermitian. In quantum theory, all observables are indeed represented by Hermitian operators, ensuring that the expectation values of these observables in physical systems are real (a system cannot have *i.e.* complex energy). In other words, imaginary numbers are useful for internal calculations, but all physical quantities (that we can measure in experiments) must have real values.

Quantum superposition and expectation values. The quantum wave-function Ψ of a given system can be used to determine the *expectation value* of physical observables of a quantum system. In general, there will be multiple solutions Ψ_n of the Schroedinger equation, each of them being a specific eigenfunction of the Hamiltonian and thus characterized by well-defined

energies E_n. Since Schroedinger's equation is a *linear* differential equation, it exhibits the property that the *superposition* of N independent solutions,

$$\widetilde{\Psi} \equiv \sum_{n=1}^{N} \Psi_n \tag{2.10}$$

is itself *also be a solution* of the same equation. On the other hand, the new solution Eq. (2.10) will in general *not be an eigenfunction* of the Hamiltonian operator $\hat{H}$, and thus will not have associated a well-defined energy E. Indeed, if we apply the Hamiltonian operator to Eq. (2.10) we find that

$$\hat{H}\widetilde{\Psi} = \sum_{n=1}^{N} \hat{H}\Psi_n = \sum_{n=1}^{N} E_n\Psi_n \neq E\widetilde{\Psi} . \tag{2.11}$$

Therefore, while a superposition of eigenfunctions constitutes a valid solution of the original Schroedinger equation, it is not an eigenfunction itself. Crucially, in the limit $N \to \infty$ the basis provided by the $\{\Psi_n\}$ eigenfunctions of an Hermitian operator is *complete*, that is, any arbitrary function can be expressed as a linear combination of the elements of the $\{\Psi_n\}$ basis.

Heisenberg's uncertainty principle. One of the central principles of quantum mechanics states that *it is impossible to specify simultaneously, with arbitrary precision, both the momentum and the position of a particle*, and is known as the *Heisenberg's uncertainty principle*. This principle is not a mere practical limitation due to for example the finite resolution of our measurement apparatus, but a *fundamental limitation* of the theory that holds true even in the case of ideal measurements. Mathematically, Heisenberg's uncertainty principle takes the following form:

$$\Delta x \Delta p_x \geq \frac{\hbar}{2} , \tag{2.12}$$

or in other words, the better the position of a particle is known, the greater the uncertainty concerning its momentum will be. Heisenberg's principle determine how well we can know at the same time specific pairs of physical observables. We define two observables Ω_1 and Ω_2 to be *complementary* if the sequential application of the corresponding operators $\hat{\Omega}_1$ and $\hat{\Omega}_2$ does not *commute*, that is,

$$\hat{\Omega}_1\left(\hat{\Omega}_2\Psi\right) \neq \hat{\Omega}_2\left(\hat{\Omega}_1\Psi\right) , \tag{2.13}$$

or in other words, the results of applying the two operators $\hat{\Omega}_1$ and $\hat{\Omega}_2$ to a generic wave-function depends on the *order in which they have been applied*. It can be demonstrated that for each pair of complementary observables there will be a relation of the form of Eq. (2.12), implying that a simultaneous measurement of Ω_1 and Ω_2 with arbitrary precision is not possible.

2.4   Summary of the lecture.

At the end of the lecture, I will summarize and recapitulate the basic concepts that I have presented during the lecture. In this case, this summary consist of a succinct overview of the *basic postulates of quantum mechanics*, which are the following:

(a) All the physical information about a quantum system is contained in its *wave-function* Ψ.

(b) This wave-function satisfies a specific equation of motion, known as the *Schroedinger equation*.

(c) The square of the wave-function $|\Psi(\{\Omega_k\})|^2$ represents the *probability density* associated to a measurement of the $\{\Omega_k\}$ set of physical observables.

(d) The wave-function Ψ must be continous, have a continous first derivative, be single valued and be squared-integrable.

(e) Observables Ω are represented by *Hermitian operators* $\hat{\Omega}$ built upon the position $\hat{x}$ and momentum $\hat{p}$ operators.

(f) Some observables are *complementary*, that is, they can not be measured simultaneously with arbitrary precision. Mathematically, their associated observables *do not commute*. Complementary observables obey then relations of the form of *Heisenberg's uncertainty principle*.

2.5   Detailed time plan.

In the table below I describe how the various contents of the lecture as well as the in-class activities are distributed among the allocated time of 50 min + 50 min. For simplicity, I will assume that the lecture starts at 11.00. In this detailed time plan there are four columns for each item, and in each column I indicate:

- The name of the activity.

- When will it start and when will it end.

- Description of the activity.

- Additional information relevant for the lesson plan.

2.6   Assessment and student feedback.

Concerning the assessment of whether or not the students have reached the learning goals of the lecture, this will be carried out using two complementary strategies.

To begin with, two days after this lecture the students will have a tutorial session (*werk-colleges*). As indicated in the revised study guide, as part of this tutorial session the students will need to complete two exercises which will then be marked by the teaching assistants. I will coordinate with the TAs to ensure that these two exercises are the most representative of the theory concepts covered during the lecture. The distribution of marks of these exercises among the students will be part of the final course assessment, and will allow me to emphasize more some of the relevant concepts if future lectures, for instance if a majority of students fail to successfully carry out an specific exercise.

In addition, as indicated in the *detailed time plan*, during the lecture the students will be engaged in three short in-class activities:

- I will check with the students how familiar are with the mathematical concepts of eigenvalue equations. I will do this by presenting them with four different eigenvalues equation and asking them using *Mentimeter* which ones they had worked with before.

- They will have to do a *quick exercise* (5 min max) in groups of two, namely solving an eigenvalue equation and determining the corresponding eigenvalues.

- Working in groups of three, the students have to apply the Heisenberg principle to determine the uncertainty on the position of a i) a car, ii) an atom, and iii) an electron. I will provide all the numerical values of the input parameters, and then the students need to compute the results and to provide the corresponding physical interpretation.

While these in-class activities are not part of the summative assessment (this is carried out during the tutorial sessions) but rather of the *formative assessment*, they will provide very useful feedback to the instructors to monitor the progress of the students and to assess

in which topics they are still somewhat week. For instance, I will ask them to hand in the solutions of the second exercise, which will provide important information about their current level of mathematics. If I find that they have a poor background in eigenvalue equations, I would make sure that during the next tutorial session they spend half of the allocated time working in eigenvalue problems under the supervision of the teaching assistants.

Name activity	Time	Description	Other details
Introduction to the lecture	11.00 - 11.05	Brief recapitulation of topics covered in previous lectures and introduction to this one, including a discussion of the learning objectives.	
The quantum wave-function and Schroedingers equation	11.15 - 11.20	See lecture contents.	Blackboard supplemented by lecture handouts.
The Schroedinger equation for a free particle	11.20 - 11.35	See lecture contents.	Blackboard supplemented by lecture handouts.
Eigenvalue equations in quantum theory	11.35 - 11.50	See lecture contents.	Blackboard supplemented by lecture handouts. Before starting, I will check with the students how familiar are with these mathematical concepts. I will do this by presenting them with four different eigenvalues equation and asking them using *Mentimeter* which ones they had worked with before.
Hermitian operators and orthogonality	12.00 - 12.15	See lecture contents.	Blackboard supplemented by lecture handouts. Before starting, they have to do a *quick exercise* (5 min max) in groups of two, namely solving an eigenvalue equation and determining the corresponding eigenvalues.
Quantum superposition and expectation values	12.15 - 12.30	See lecture contents.	Blackboard supplemented by lecture handouts.
Heisenberg's uncertainty principle	12.30 - 12.45	See lecture contents.	Blackboard supplemented by lecture handouts. Short *in-class activity*: working in groups of three, the students have to apply the Heisenberg principle to determine the uncertainty on the position of a i) a car, ii) an atom, and iii) an electron.
Summary of the lecture	12.45 - 12.50	Summary of the main concepts discussed in the lecture and review of the most important take-away lessons for the students. Brief discussion of the topics to be covered in the subsequent lecture.	The students can ask general questions about the topics covered in the lectures. After each lecture, I stay up to 30 min in the lecture room to answer these and related questions for the students.

3 Lesson Plan II

HC11: Molecular spectroscopy and electronic transitions

3.1 Overview of the lecture

In this lecture, I will present the basic concepts underlying electronic transitions in *p-electron conjugate systems*, the Franck-Condon principle, the physics underlying the phenomena of *fluorescence* and *phosphorescence*, as well as the basic principles of operation of a *laser*. I will also present an explicit application of these ideas in the medical context, namely the *photo-dynamic therapy* (PDT), which is used for example in a number of cancer therapies.

The *learning goals* of this lecture are:

(a) Understanding and applying π-π^* electronic transitions in molecules.

(b) Understanding which electronic transitions can take place for either absorption or emission of a photon while the atomic nuclei are at rest (the Franck-Condon principle), including the mathematical description and implications of absorption and emission spectra.

(c) Understanding and applying the principles of fluorescence and phosphorescence.

(d) Understanding the basic principles that underlie the operation of a laser, such as the concept of population inversion.

3.2 Resources and preparation

The contents of this lecture will be based on the course textbook, Atkins and de Paula, *Physical Chemistry*, 10th edition, Chapter 10. They should read the relevant sections of this chapter before the lecture. In addition, the lecture notes (handouts) will also be made available before the lecture on Canvas, and the students will be encouraged to take a look at them beforehand.

Given the nature of the course, it is very difficult to follow the lectures of the latest part of the course without a proper grasp of the concepts presented in the previous lecture. With this motivation, I will ask the students to read beforehand the lecture notes of the two previous lectures (HC9 and HC10) and ask me before the class if they have any question.

3.3 Topics to be covered during the lecture

In the following I indicate that various topics that will be covered during the lecture. After that, I indicate in a table below the amount of time that should be devoted to each topic, as well as to the additional in-class activities that will be carried out during the lecture. Here I also indicate the visual material that will be shown during the lecture, in particular those graphs that are used to illustrate the consequences of the theory concepts that have been introduced.

Electronic transitions in molecules. In the previous lecture we studied the transitions between different vibrational states of a molecule. We now consider instead the *electronic transitions* that take place between different electronic states of a molecule. As opposed to vibrational transitions, which were associated to *infrared frequencies*, electronic molecular transitions take place mainly in the *visible and ultraviolet* regions of the electromagnetic spectrum, and therefore, among the many important properties of these transitions, they are also responsible of the *color* of materials and substances.

I will recall some of the concepts that the students have seen in previous lectures, in particular the fact that in molecules, under the right circumstances, the electrons might become *de-localized* by means of the overlap between individual atomic orbitals, that is, they cannot be assigned to any of the specific components of the molecule. The strongest type of *chemical covalent bonds* in molecules are known as σ-bonds, formed by a head-on overlapping between atomic orbitals leading to a molecular orbital. The key property of this bond is that the resulting orbitals are *rotationally symmetric with respect to the bond axis*. Another important type of molecular bonds are the so-called π-bonds, covalent chemical bonds where two lobes of one atomic orbital overlap with the two lobes of another atomic orbital, resulting in the bonding between the two atoms. In Fig. 3.1 we show how a π-bond in a di-atomic molecule is formed by the partial overlap between atomic p-type orbitals.

Understanding electronic molecular transitions. Next I will present some additional facts that are important for the understanding of the physics underlying electronic transitions between molecular orbitals, including:

- In molecular orbitals, the *conjugation length* is defined as the length of the orbital resulting from the partial overlap of atomic p-orbitals.

- In some circumstances, an electron might transition between a n orbital of an *auxochrome* to the π^* orbital of a *chromophore*. In this transitions, the larger the conju-
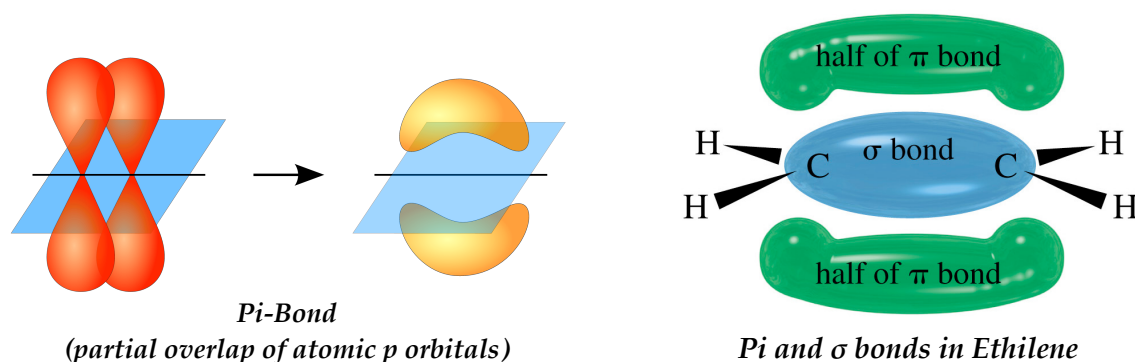
Molecular Orbitals

Figure 3.1: Left plot: a π-bond in a molecule is formed by the partial overlap between atomic p-type orbitals. Right plot: the bonding structure of ethylene, C_2H_4, showing a σ bond between the two C atoms (rotationally symmetric with respect to the bond axis) and the two halves of the π bond arising from the p atomic orbitals.

gation length, the larger the *extinction coefficient* that determines how strongly this specific molecule will absorb light of a given wavelength.

- There is a direct connection between the value of the dipole moment transition matrix element μ_{fi} and the extinction coefficient $\epsilon(\nu)$ for light of a given frequency, that determines how strongly this molecule does absorb light of this specific frequency.

The Franck-Condon principle. This important principle describes the transitions in which a *simultaneous* change in the vibrational and electronic states of a molecule takes place, due to the emission or absorption of a photon of the appropriate energy. It states that since nuclei are so much more massive than electrons, $m_e \ll m_N$, *electronic transitions* between different quantum states take place at much shorter time-scales that those for which the nuclei can respond, therefore the *vibrational transitions* take place at slower rates. In other words, the probability of an *electronic molecular transition* is the highest where the *relative separation between two atomic nuclei* is unchanged. This phenomenon is thus also known as a *vertical transition*, since in a (r, E) plane the transition takes place vertically along the y axis, as shown in Fig. 3.2.

Dipole matrix element for vibronic transitions. In order to compute the matrix element for the electric dipole moment of such a vibronic transition, we need to take into account the sum of electronic and of nuclear contributions to the total molecular dipole moment operator,
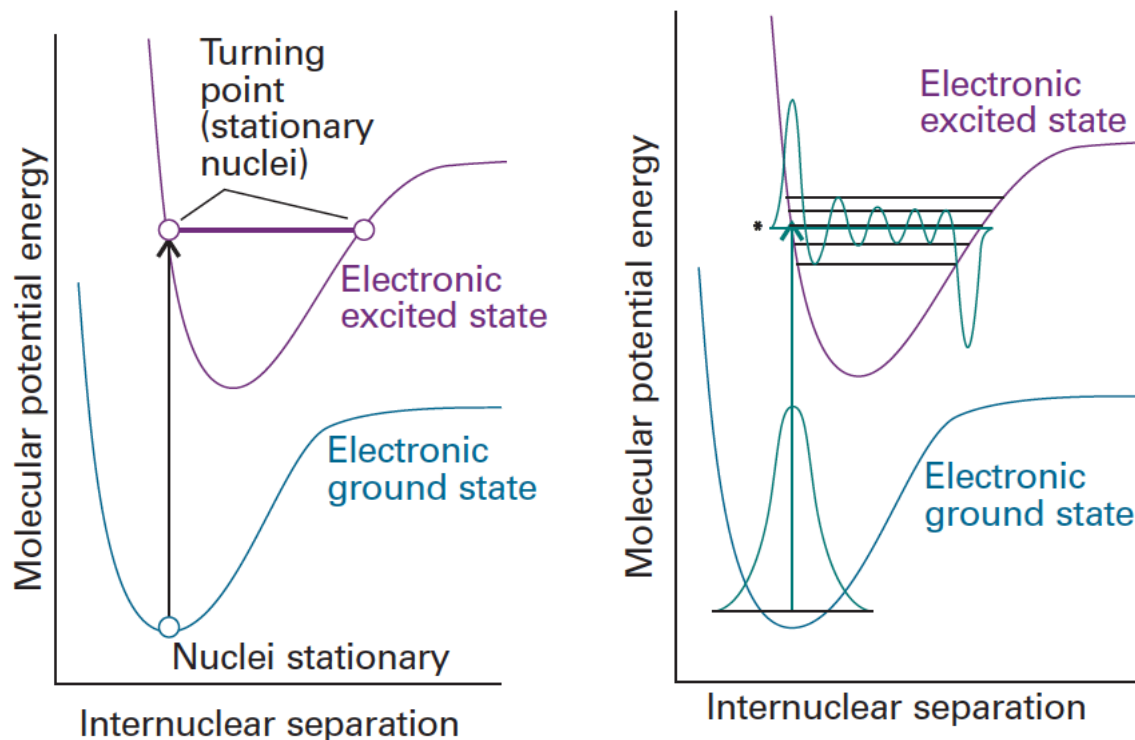
Figure 3.2: Schematic representation of the molecular potential energy (Morse potential Eq. (**??**)) for the ground and the excited electronic states in a molecule. Left plot: according to the Franck-Condon principle, the most intense vibronic transitions takes place between the ground vibrational state in the electronic ground state to to the vibrational state lying immediately above it in the electronic excited state, in a way that the *inter-nuclei separation* is kept constant. Transitions to other vibrational states also occur, but this lower intensities. Right plot: in the quantum mechanical description of the FC principle, the molecule undergoes a transition to the upper vibrational state that most closely resembles the vibrational wave-function of the vibrational ground state of the lower electronic state. The two wave functions shown here exhibit the greatest overlap, and hence the matrix element for the transition probability among them is the highest, corresponding to a transition with fixed inter-nuclear separation.

that is

$$\hat{\vec{\mu}} = -e \sum_j \vec{r}_j + e \sum_I Z_I \vec{R}_I \,, \tag{3.1}$$

where j runs over the electrons and I over the nuclei in our molecule, and Z_I is the total positive charge of the nucleus I. If we now define

$$S(\nu_f, \nu_i) \equiv \int \Psi^*_{\nu_f} \Psi_{\nu_i} d\tau_\nu \,. \tag{3.2}$$

it can be shown that the rate for a vibronic transition that involves simultaneously the change in the electronic and vibrational states of a molecule will be proportional to the

Franck-Condon factor,

$$|S(\nu_f, \nu_i)|^2 \,, \tag{3.3}$$

which states quantitatively what was qualitatively illustrated in Fig. 3.2, namely that the rate for vibronic transitions is maximal when the vibrational wave functions in the ground and excited electronic states resemble the most.

Fluorescence and phosphorescence phenomena. Next, I will move to describe two important phenomena related to light emission by molecules. *Phosphorescence* is the *slow emission of light* in molecules, taking place in an interval of *microseconds or more*. And *fluorescence* is the *fast emission of light* in molecules, taking place within a time interval of *nanoseconds* or less. Therefore, these two phenomena related to light emission in molecules have time scales that differ by several orders of magnitude. To explain the quantitative differences between these two phenomena, I will use a *Jablonski diagram*, which schematically indicates the transitions that can take place starting from an excited state within a molecule. In Fig. 3.3 we show the schematic representation of the fluorescence and phosphorescence phenomena by means of a Jablonski diagram. By doing this, we should be able to show that the key property of phosphorescence is that following light absorption, the subsequent re-emission takes place at a lower intensity for up to several hours after the original excitation. Therefore, it is a very slow transition.

Operation principles of lasers. The use of lasers is ubiquitous in spectroscopy, as well as in many forms of microscopy and in a *wealth of medical applications*. Therefore, it is important to understand how a laser works. The name *laser* was originally an acronym of *Light Amplification by Stimulated Emission of Radiation*, since it is a device that *amplifies the intensity* of the incident electromagnetic radiation. In this part of the lecture I will illustrate in a qualitative way the operation principles of lasers. Specifically, I will show that a necessary condition for *lasing* is achieving *population inversion* in the system, that is, a situation such that in thermal equilibrium the population of excited states is higher than the population of lower energy states. Only under this condition it will be possible to achieve more stimulated emission than stimulated absorption, and this achieve amplification of the incident radiation intensity. To exemplify these theoretical concept, I will use Fig. 3.4 for the discussion, which illustrates the basic operation principles of lasers.
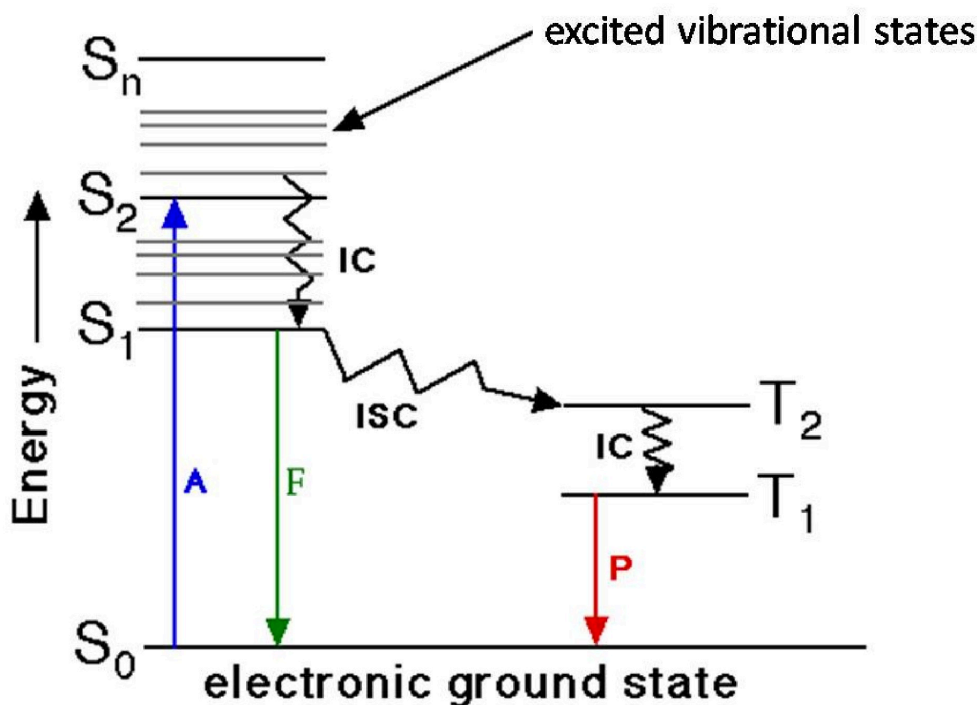
Figure 3.3: Schematic representation of the fluorescence and phosphorescence phenomena by means of the *Jablonski diagram.* In this diagram, A indicates the absorption of a photon, F and P represent the fluorescence and phosphorescence transitions respectively, S and T denote singlet and triplet states, and finally IC and ISC label the internal conversion and the inter-system crossing respectively.

Applications to medical science: Photodynamic Therapy. PDT is a representative example of a medical application which is based on the optical transitions between different molecular electronic states. PDT, also known as *photo-chemotherapy*, is a form of photo-therapy involving light and a photosensitizing chemical substance, which in conjunction with molecular oxygen can eliminate cancerous tissue. In this part of the lecture I will explain how PDT works, connecting with the more theoretical concepts introduced earlier in the lecture. To explain why PDT is useful for medical applications, we start from a molecular singlet state, with two paired electrons (opposite spin) in the same electronic quantum level. This level will be the HOMO, the Higher Occupied Molecular Orbital, as illustrated in Fig. 3.5. Using laser radiation, an electron is excited to first the LUMO orbital and then via an inter-system crossing it ends up in its first excited triplet state ^3P. The resulting state photosensitizes the formation of an excited singlet state of O_2, $^1O_2$, which are extremely reactive and destroy cellular components. This can be used to target cancerous cells and destroy them without affecting the the meantime healthy tissue.
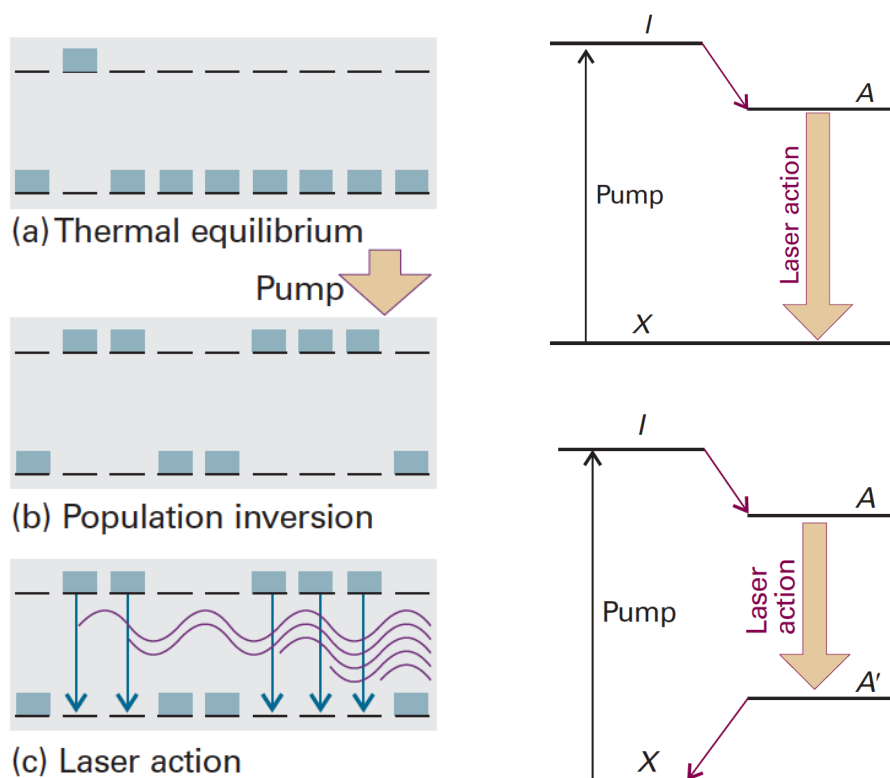
Figure 3.4: Left plot: the operation of a laser is based on the principle of *population inversion*: starting from a system in thermal equilibrium, obeying Boltzmann statistics and thus where the population of the excited state is smaller than that of the ground state, a *pumping system* increases the population of the excited state until it becomes larger than that of the ground state. In these conditions, stimulated emission will dominate over absorption and this the laser will indeed enhance light intensity. Right plot: The schematic operation of a three-level (upper diagram) and four-level (lower diagram) laser, where we indicate the specific transition that is responsible for the lasing.

3.4   Summary of the lecture

At the end of the lecture, I summarize and recapitulate the basic concepts that I have presented during the lecture. For this lecture, the most important take-away messages that the students should recall are the following ones:

(a) The absorption of light (visible and UV) in biological molecules takes place predominantly by means of $\pi \to \pi^*$ transitions in p-conjugated electron systems.

(b) A larger p-electron conjugation length leads to absorption at longer wavelengths, that is, at smaller photon energies. This is explained by the reduced electron confinement for large conjugation lengths.
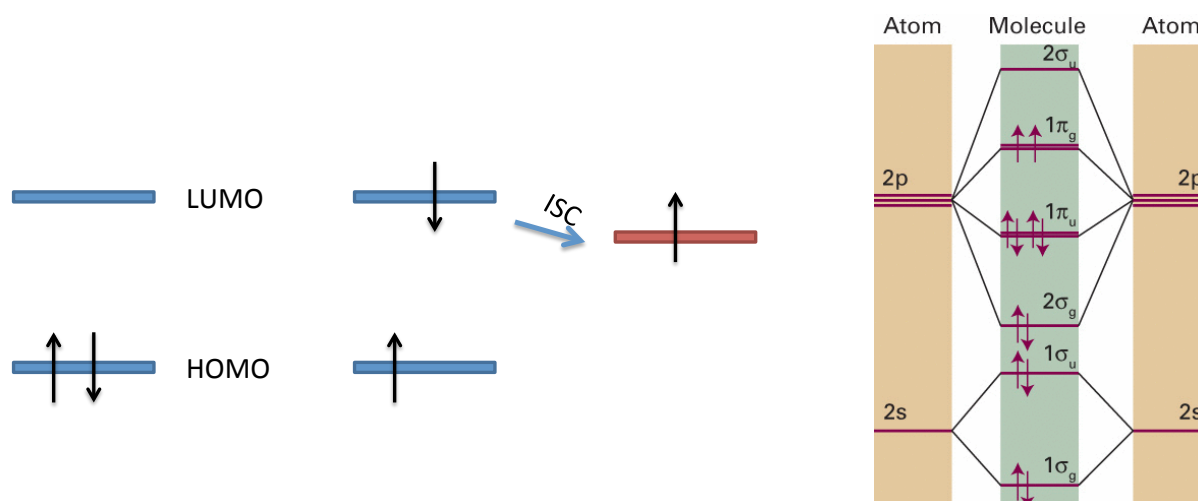
Figure 3.5: Left plot: the basic molecular electronic transition in *Photodynamic Therapy* is the one from a singlet state with paired electrons to a triplet state where the two electrons have unpaired spin via an inter-system crossing. Right plot: schematic representation of the molecular orbitals in the O_2 molecule, where the $2s$ orbitals form two σ-bonds and the $2p$ orbitals form two σ and two π bonds.

(c) Symmetry considerations are important when determining whether or not an given optical transition is possible within a specific molecule.

(d) The Franck-Condon principle explains the transitions in which a *simultaneous* change in the vibrational and electronic states of a molecule takes place, the so-called *vibronic transitions*.

(e) The Einstein coefficient for spontaneous emission determines the radiation lifetime of a molecule τ_R, which in general is different (larger) than its total lifetime.

(f) The fluorescence lifetime τ_F is usually shorter than the radiative lifetime τ_R due to competing processes that de-populate the excited states.

(g) The phosphorescence phenomenon is explained by the long-lived emissions from a triplet excited state to a singlet ground state.

(h) The light amplification achieved in a laser is based on the concept of *population inversion*.

(i) The Photodynamic Therapy is an representative example of a medical application based on optical transitions in biomolecules.
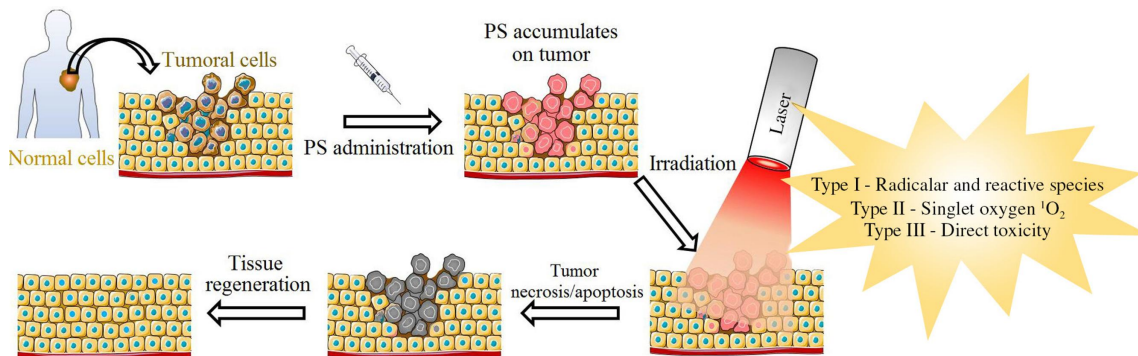
Figure 3.6: In photo-dynamic therapy, a photo-sensitive (PS) molecule is injected on the patient and accumulates on tumor. The subsequent irradiation activates a chemical reaction which creates reactive oxygen molecules $^1O_2$ which destroy the cancerous tissue.

3.5   Detailed time plan.

In the table below I describe how the various contents of the lecture as well as the in-class activities are distributed among the allocated time of 50 min + 50 min. For simplicity, I will assume that the lecture starts at 11.00. In this detailed time plan there are four columns for each item, and in each column I indicate:

- The name of the activity.

- When will it start and when will it end.

- Description of the activity.

- Additional information relevant for the lesson plan.

Note that the general format for this detailed time plan is the same as for the first lesson plan.

3.6   Assessment and student feedback.

Concerning the assessment of whether or not the students have reached the learning goals of the lecture, this will be carried out using two complementary strategies.

To begin with, two days after this lecture the students will have a tutorial session (*werk-colleges*). As indicated in the revised study guide, as part of this tutorial session the students will need to complete two exercises which will then be marked by the teaching assistants. I will coordinate with the TAs to ensure that these two exercises are the most representative

of the theory concepts covered during the lecture. The distribution of marks of these exercises among the students will be part of the final course assessment, and will allow me to emphasize more some of the relevant concepts if future lectures, for instance if a majority of students fail to successfully carry out an specific exercise.

In addition, as indicated in the *detailed time plan*, during the lecture the students will be engaged in three short in-class activities:

- I will check with the students how familiar are with the concept of wave function overlap. I will do this by presenting them with three different wave function configurations, and asking them using *Mentimeter* which ones do they expect to lead to a bigger matrix element. In other words, by looking at different wave function overlaps they need to understand which cases will have a largest transition probability.

- They have to do a *quick exercise* (5 min max) in groups of two, namely looking at two sets of electronic transitions and trying to guess which one will have the largest lifetime. This involves using their understanding how which transitions between electronic levels are allowed by symmetry principles, and which ones are disfavoured from physical considerations.

- Working in groups of three, the students need to propose a possible efficient medical protocol based on using PDT to help a patient with stomach cancer. This exercise aims to help the students to apply what they have learned in the lecture to an realistic application, as if they were working in a medical environment.

While these in-class activities are not part of the summative assessment (this is carried out during the tutorial sessions) but rather of the *formative assessment*, they will provide very useful feedback to the instructors to monitor the progress of the students and to assess in which topics they are still somewhat week.

For instance, I will ask them to hand in the solutions of the second exercise, which will provide important information about their understanding of the nature of the allowed electronic transitions between molecules. If I find that they have a poor background in this, for example if they get confused between the *fluorescence* and the *phosphorescence* phenomena, I would make sure that during the next tutorial session they spend half of the allocated time working in problems related to electronic molecular transitions under the supervision of the teaching assistants.

Name activity	Time	Description	Other details
Introduction to the lecture	11.00 - 11.05	Brief recapitulation of topics covered in previous lectures and introduction to this one, including a discussion of the learning objectives.	
Understanding electronic molecular transitions.	11.15 - 11.20	See lecture contents.	Blackboard supplemented by lecture handouts.
The Franck-Condon principle.	11.20 - 11.35	See lecture contents.	Blackboard supplemented by lecture handouts.
Dipole matrix element for vibronic transitions.	11.35 - 11.50	See lecture contents.	Blackboard supplemented by lecture handouts. Before starting, I will check with the students how familiar are with the concept of wave function overlap. I will do this by presenting them with three different wave function configurations, and asking them using *Mentimeter* which ones do they expect to lead to a bigger matrix element.
Fluorescence and phosphorescence phenomena.	12.00 - 12.15	See lecture contents.	Blackboard supplemented by lecture handouts. Before starting, they have to do a *quick exercise* (5 min max) in groups of two, namely looking at two sets of electronic transitions and trying to guess which one will have the largest lifetime.
Operation principles of lasers.	12.15 - 12.30	See lecture contents.	Blackboard supplemented by lecture handouts.
Applications to medical science: Photodynamic Therapy.	12.30 - 12.45	See lecture contents.	Blackboard supplemented by lecture handouts. Short *in-class activity*: working in groups of three, the students need to propose a possible efficient medical protocol based on using PDT to help a patient with stomach cancer.
Summary of the lecture	12.45 - 12.50	Summary of the main concepts discussed in the lecture and review of the most important take-away lessons for the students. Brief discussion of the topics to be covered in the subsequent lecture.	The students can ask general questions about the topics covered in the lectures. After each lecture, I stay up to 30 min in the lecture room to answer these and related questions for the students.