student summaries and exam question suggestions
Setting the stage

These pages contain student summaries for the module **Setting the stage**, *as well as student suggestions for exam questions on this module. You can use these pages as a study help for this module. The summaries can help you to see the highlights of this module from different points of view. The questions can challenge you to think about the content. If you take the exam, then some of the questions suggested this year will be included in the exam. The contributions suggested this year are* are printed in color. *The ones in black were contributed in previous years.*

1. student summaries

- Ab initio means to obtains properties of a system trough fundamental equations. In that order quantum physics uses the Schrödinger equations. A solid is a positive nuclei and negative electrons electromagnetically interact with each other. Even though we know the equations that have to be solved, actually solving them takes longer than a lifetime. That is why we use quantum physics simulations to find properties by trial an error. But scientists in the field have a huge privilege, because their main tool (computer) gets exponentially better with the years.
- Quantum based materials calculations are simulations bases on fundamental physical laws
- This course will show methods to solve problems regarding material science. For this, a computational approach is used to calculate the properties of materials. To do calculations, many different softwarepackages can be applied on hardware that keeps increasing in strength. The course will look at solids as a combination of positive nuclei and negative electrons, that interact according to the rules of qauntummechanics.
- What ab initio is, what a solid is, why we do these calculations and their advantages and disadvantages.
- We should remember the importance of calculation of solid properties from first principles, the definition of ab initio and the definition of a solid.
- Formal system of solid and treat solid as a collection of charges not as atom.
- Ab initio means that a certain theory starts from basic formulas/axioms and then can predict about all kinds of experiments in its field. Do not take this too far, quantum should only be used when it makes sense treat things quantum mechanically. Also, sometimes it's not realistic to solve everything exact in a quantum way, that would take an infinite amount of time. Therefore we make approximations. Simulation has become more and more important and its breakthroughs will increase (computationalo power doubles every 2 years). Simulation is not the same as theory.
- Mainly understanding what ab initio methodes are how/why these are used for modern material research. It is also good to understand the current situation of computational resources that are available in the world and for you personally.
- A solid is a system consisting out of nuclei and electrons, and not out of atoms.
- I think an essential aspect is the understanding what ab initio actually means, especially in the context of materials Science, as well as the main problem arising when trying to use ab initio methods or quantum mechanical approaches in the description of material properties.
- I think the main takeaway from this chapter is the fact that simulation can help a great deal in material science, speeding up research that would take a long time or even be impossible when doing only experimental research.
- How is the ab-initio way different from other ways to understand nature.
- I think the massive amount of possibilities that computation opens, especially in synergy with theory and experiment.

  The fact that, without doing anything, computational power keeps increasing.

- Solids are made up of positive and negative charges like nuclei and electrons interacting via the laws of quantum mechanics. The idea about abinitio comes from solving problems from first principle which for our case is the Schrodinger equation.

- Computational ab initio methods are an area of science that use the most basic principles of a problem to develop solutions. In materials science, this is related to the solution to the Schrodinger equation, but the time required to solve this exactly is impractical, creating the need for approximations.

- Computational methods is an always evolving field and will produce better, more accurate and faster results with each passing year. However, the importance of experiments cannot be understated as it is as important. Secondly, the concept of 'atoms' in the framework of DFT doesn't work so well, instead ions and nuclei and their interactions are the focal point. Thirdly is that it is important to stress that DFT in itself is a faithful transformation of a very complex problem into a 'simple' one where the most difficult part is finding the XC functional. It by itself remains an ab initio (first principles) model

- The definition of a solid, the reason we use computation and the difference with theory, the problem with slow computations,

- The definition of solid, Advantages

- We should appreciate the new possibilities the simulation brings to materials science and condensed matter physics. Also, we should distinguish between theoretical physics and simulation as these are fundamentally different but both are important for the progression of science and technology. We should also have a good understanding of ab initio method and what it means.

- To approach a material (definition of a solid) in quantum physics, with just the component charges (nucleus and electron) and their interactions.

  To understand the limitations of DFT calculations. Not to become too ambitious.

  The importance of ab-initio models and how they can explain everything related to a system just because they are the most fundamental definition of a system.

- First a definition of a formal sistem, which is basically a description of steps or ideas to be clear to explain a physical phenomena. I also learned about composition of a crystal where atoms are not seen anymore as atoms but a density of electrons. More important the difference between the theoretical and simulation fields, where the first one is the mathematical description of a physical phenomena observed in nature while the simulation is using that mathematics and changing variables to see how it changes.

- •A solid is a cllection of nuclei and electrons that are interacting under the electromagnetic interaction and follow thr fundamentals of quantum mechanics. •A Material is more than just a solid, crystal structure + microstructure. •The goal of a material scientist is knowing the tools to bring new way of doing materials science into practice. •Therory is building new science, then experiment comes to validate that theory, then simulation comes to perform more tests and trials

- for the purposes of this course, we should not describe a solid by it's atoms, but rather by it's nuclei and electrons

- In this lecture we have defined concepts like an ab initio model, a formal system and a solid. We have also discussed what a material scientist is and what place computational physics takes in the experiment vs theory structure. One should know the possibilities that have opened up to scientists with the introduction of this relativily new branch of science and the advantages and disadvantages associated with it. Finally one should also keep in mind that future advancements in the resources used by a computational scientist (hardware/ software) will open up even more opportunities in this field.

- The strengths and limitations of computational simulations. The definition of a solid. What ab initio implies.

- Difference between theory, simulation and experiment and the definition of a solid

- Solids are a collection of positive and negative charges, with electromagnetic interactions that obeys the law of quantum mechanics. Being an ab initio study, quantum mechanics can predict all the properties of solids, the only limitation is time
- A formal introduction to the ab initio/quantum description of solids was given, including a description of formal systems in physics and their usage. The quantum nature of solids was discussed and ways to describe such quantised behaviour, in terms of both hardware and software, were laid out.
- We should remember what an ab initio model is and how fundamental theory in QM has already been developed. Also that In solid, we do not deal with atoms but nuclei and electrons. And that we cannot define solid by electromagnetism only, quantum physics is also required. The differences between solid and materials(defects, grain boundaries, etc.) are also important to remember.
- NaT
- In DFT, the fundamental insight of the Schrödinger equation is solved numerically for a certain situation, i.e. a number of atomic nuclei and a number of electrons. One of the goals is to approximate the ground state of the system and its associated energy, but many other properties can be calculated as well, including some macroscopic properties. Only thanks to enormous advances in computing power has this beome a viable way to derive information.
- Notion of need of computational calculation and simulation for materials, why ab initio is important, etc.
- Understanding solids in quantum mechanics will require ab-inito methods which will help, let's say material scientists, to solve Schrödinger equation. Thus calculating a material systems properties. Its a way to apply theoretical knowledge in simulations via methods such as Density Functional Theory. It requires supercomputers for complex problems and practical knowledge of software's such as Quantum Espresso.
- The Schrödinger equation is the fundamental equation of quantum mechanics. It's the basic equation that tells us how matters behave. This means that we know everything about a certain solid if we can solve the Schrödinger equation of that solid. However, we are not always able to do so in a sufficient small time scale although we know the algorithms to solve the Schrödinger equation. Otherwise, this would offer a lot of advantages. For example, A material scientist could use quantum physics for material design in the same way as a construction engineer uses classical mechanics for construction work. Nevertheless, our computers become twice as good every two years, so maybe in the future this is just reality.
- That a solid is not defined as a collection of atoms, but of positive nuclei and negative electrons. So the definition of a solid. The maturity of materials science and that time is the most important limiting factor. The role of simulation in relation to theory and experiment.
- The evolution of the computing power: this doubles every year. This is a very strong growth. Classical mechanics can be exactly calculated and is an ab initio model. Quantum physics isn't able to be calculated exactly and is also an ab initio model.
- Solids are inherintly quantum mechanical, for which the equation is known: the Schrödinger equation. Starting only from this equation is called the ab initio way. This is certainly possible, but can be very time consuming. Luckily computers get twice as fast every two years (Moore's law). For some problems, this is still way faster than designing and testing materials in the lab.
- Defination of solid, first principle,
- The difference of theory, experiment and simulation. The theory is originated from experiment, the simulation is based on theory which is no major flaw after many extreme experiment. Ab initio simulation is make the difference between construction mechanic and materials engineering.
- What the ab-initio way is and how computational is different from theoretical.

- We should remember the problem with the application of quantum mechanics and how the computation can help us out in this regard(up to some extent). We should know about the hardware of the system which we are using and also about the fastest computing facilities which are available to us and around the world. From conceptual point of view we should also know the power of an ab initio way of solving a problem and how to categorise any system into ab initio way.
- The idea that material properties can be obtained by calculating Schrödingers equation and that solids should be discussed in the point of view of quantum mechanics . Also the idea that computers play an important role in material science. And the difference between theory and computation.
- I think that the essencial things are the definitiva of ab-initio model, the definition of a cristal and the role of computational simulation for the field of material science.
- What is an ab initio model and why is computational mat. phys. one? Defintion of a solid
- How to discriminate which models are an ab initio and which aren't. The definition of a solid. Advantages of treating solids by quantum physics.
- I understand that we will study solids using quantum mechanics and modelling them as a regular of positive nuclei and electrons. Our main task is to solve Schrodinger's equation in this system but this require several approximations due to the complexity of the task.
- In the context of computational material physics a solid should be regarded as a collection of positively charged nuclei and negatively charged electrons, rather than a rigid collection of stationary atoms. Materials can be designed based on ab initio quantum calculations if the required computing power is available.
- 1) Solid is a collection of nuclei and electrons. 2) Computational approaches are now a standard toolset in materials physics.
- Definition of a solid (hint: don't mention atoms) Possibilities of ab initio What makes a theory ab initio?
- Materials (solid quantum systems) can be created from thought using quantum ab initio methods, although this is not always computationally straightforward. One can do this with certain hardware and lots of different software.
- Classical physics is not enough to screen motions in atomic scale, so that reason we need to use ab-initio. Mechanical equations also can not solve that problems in atomic scale, we should considet schrödinger always.
- the difference between theoretical ,experiential and simulation works
- You need quantum mechanics to properly describe solids. The aim of density functional theory is to accurately simulate materials to predict their properties without a need for experiment. Density Functional Theory is an ab initio method (a small number of axioms can be used to yield experimental observables). Theory and simulation are separate activities, theory develops equations and simulation solves equations to get data.
- - Quantum physics is an ab initio method, due to it having a "basic" formula (Schrödinger) - Solids cannot be seen as atoms grouped together in this course - Quantum physics is not theory because all the formula have been found and experiments have been practiced to verify them
- To learn from this chapter: what are the problems of quantum mechanics compared to classic mechanics. Differences between computational and theoretical methods. There are a lot of different software programs to solve Schrödinger's equation.
- We are doing a simulation of mature theoretical works on solids which has limitations itself to improve materials database.
- It is definately important to understand when a theory is ab initio and when it isn't, as it brings understanding of the working principles of DFT methods.

- What the future holds for materials and advanced in the application of materials to solve problems. The basic understanding of what ab nitio is about. The appropriate hardware and software to use in this course.
- I will for sure remember the definition of the formal system ad ab inito.
- I should remember solids are not to be viewed as groups of atoms, but as groups of interacting nuclei and electrons instead. I can understand how to calculate total energy of a unit cell as shown in the video. It is also important to realize the problem with creating materials "from thought" is not the theory, we have it already fully figured out, but rather the computational difficulty.
- Solids are quantum Systems and should be treated quantummechanically. When we're making calculations to find the Properties of the solids, we're not doing theoretical Physics, but computational Physics because we're not making a New Theory. There is however a problem, namely that it takes too much time to Solve the Schrödinger equation for a few particles.
- Why it is really handy to use a DFT model to obtain knowledge about certain material properties
- The meaning of formal system and the meaning of a solid in quantum physics
- Definitions of a solid and an an initio method.
- Classical physics is not enough to screen motions in atomic scale, so that reason we need to use ab-initio. Mechanical equations also can not solve that problems in atomic scale, we should considet schrödinger always.

2. exam question suggestions

- Why in this area a solid cannot be described with atom?
- Why are ab initio calculations considered simulations?
- What is the difference between theory, experiment and computation and how does a scientific field evolve using these different study-techniques?
- Why don't we just calculate all material properties with DFT code.
- Explain why a solid can or cannot be described using quantum/classical mechanics and give the definition of a solid, and justify why this is a good definition.
- In which cases we should not use ab initio model?
- What would you say if your mother asks why you need to study classical mechanics and quantum mechanics both? Isn't one of them outdated?
- Formulate the contribution of ab initio methodes in contemporary material research.
- What is an "ab initio" model?
- Describe a solid in terms of quantum mechanics
- What is the difference between theory and simulation as research fields?
- What is the definition of a solid, as a quantum system?
- What's a fundamental advantage computational methods have compared to experimental ones?
- What are solids and why classical mechanics does not allow molecules to form
- In what way can ab initio simulation and theory be differentiated?
- What are the reasons the use of DFT has undergone such a drastic revolution these past years?
- How would you describe a formal system?
- What is Solids as quantum system and difference between theory vs computation?

- why are solids quantum systems and not classical?
- What is the meaning of an initio calculations and what are important in quantum material simulation?
- -What is the different between a solid and a material? -clarify the different between theory, experiment and simulation. - What is the role of a materials engineer?
- What does DFT stand for?
- What is an ab initio model? Choose a branch of physics and explain why it does or does not constitute an ab initio model.
- What are the strengths and limitations of computational simulations.
- Name three stages of development for a scientific field. State how each stage uses theory, experiment and simulation and give an example of a field in each stage.
- What is the limitation of quantum mechanics
- Why must a solid be treated by means of quantum physics (as opposed to quantum physics)? Motivate the answer by using an appropriate formalism and indicate how you would computationally describe a solid in practice.
- Find total energy of an FCC cell of helium atoms.
- NaT
- What is/isn't an ab initio method? How would you do an ab initio calculation for this specific physical problem?
- Explain computation in your words connecting it with quantum systems, theories, and ab inito way.
- True or False: [example] is an ab initio model? Why do you think it is/isn't an ab initio model?
- Give the definition of a solid, explaining every part of the definition and its importance. How would this definition differ from the definition of a fluid?
- Why is computational physics such a growing field?
- What does "ab initio" mean? Give two examples.
- Define solid
- Describe in brief how solids behave as a quantum system .
- What are the basic underlying concepts of ab initio way?
- What is the definition of a solid?
- Briefly describe how computational materials physics can take part into developing new applications
- Why, in the definition of a solid, we say that there are no atoms?
- When we were setting the stage for this course, we introduced the definition of a solid to be used for the rest of the course. Please explain what is a solid.
- Explain the difference between theory and simulation. Formulate a sound criteria to distinguish these two activities.
- Why is quantum physics essential for treating solids?
- Give an example of a theory that is not ab initio.
- What is a solid and how can we describe them? (In theory and practically)
- Can we apply ab-initio equations to macro scale?

- Define an ab initio method, give an example of an ab initio technique and a non-ab initio technique (explain your reasoning)
- Explain why quantum physics is an ab initio method and what other ab initio methods do you know (and which formula are important)
- What are the problems of quantum mechanics compared to classic mechanics?
- Discuss the difference of molecular dynamics and dft methods and suggest where we would benefit from them the most?
- Can DFT be applied to liquids? Argument why or why not. In case your answer is yes: Give an example of a property of a liquid that could be determined using DFT and give the name of the corresponding ab initio theory.
- Please create a formal system then can be used for a physical system.
- Explain why you cannot perceive a solid as a group of atoms (with help of hydrogen - atom, molecule, crystal)
- What's the advantage of treating solids by quantum Physics?
- In which stage of its growth (infancy, teenager, mature) is material science situated? Explain why.
- How can we differentiate a solid from a liquid with quantum definition?
- If you were to think of your ethical philosophies as an ab initio method, on what axioms would they be based?
- Can we apply ab-initio equations to macro scale?
- What is the difference between theory and computation? Illustrate using the case of quantum physics.