Study guide – quantum mechanics

These are mostly concept questions and/or memorizing questions. You have also to be able to solve numerical problems. The assignment of quizzes and exams may differ in a given year for the list below.

Based on the textbook "Physical Chemistry" of T. Engel and P. Reid.

Chapter 12 – from classical mechanics to quantum mechanics

Class 1 – blackbody radiation

-) What were the main results of the blackbody experiment?
-) What systems can be described by Planck's blackbody equation? Name three examples.
-) How does a plot of the energy density vs. wavelength look like for the blackbody? Include three curves for different temperatures. Label the plot.
-) How does the total energy of a blackbody scales with temperature?
-) What is a density? Why are densities used in quantum mechanics?
-) How does a plot of the energy density vs. frequency look like for the blackbody? Include three curves for different temperatures. Label the plot.
-) $A \sim B^2$, what does the symbol ~ imply?
-) What does a pizza oven and the cosmos have in common?
-) An ultraviolet catastrophe is a concept from star track that does actually not exist. True/false?
-) What did Wien discover?

Class 2 – photo effect

-) Describe the photo effect by means of a simple drawing of an experimental set up.
-) What are the main experimental results of the photo effect experiment?
-) What are the expectation from classical physics?
-) How did Einstein explain the photo effect? What was the main idea?
-) What have billiard playing and running a photo effect experiment in common?
-) What is a photon?
-) Is light a particle or a wave or what?
-) What is the energy of a photon?
-) What is the particle – wave duality?
-) What is the electronic work function
-) What is Einstein's equation to describe the photo effect?
-) How to measure Planck's constant
-) The photo electric effect is used today as a spectroscopic tool. Explain.

Class 3 – de Broglie's matter waves

-) Would you see diffraction effects if an elephant is walking through a door? Why?
-) Is the de Broglie wavelength large or small for a macroscopic object?
-) Write down the wavelength of matter
-) What could be considered an experimental proof of de Broglie's theory
-) Do you see diffraction pattern when shooting with an electron beam at a crystal?
-) Does this also work with Kr atoms? Explain?
-) What is the double slit experiment all about? What results are consistent with a particle model? What is consistent with a wave model?

-) What was the main conclusion of the double slit experiment?

Class 4 – Bohr model (briefly since you have seen this before)

-) What is an emission spectrum?
-) What is an absorption spectrum?
-) Sketch qualitatively the emission pattern of a gas such as helium or hydrogen
-) List Bohr's postulates
-) What was the main accomplishment of Bohr's model?
-) The Balmer series revers to good luck in a row when playing lottery? Yes/no.
-) What is the Lyman series?
-) What are stationary states in the framework of Bohr's model?
-) Does an electron emit radiation in a stationary state?
-) Only the energy is quantized but certainly not the angular momentum. Yes/no.
-) The emission lines of Helium are evenly spaced in the frequency domain. Yes/no.
-) Hydrogen and deuterium will result in the same emission spectra? Yes/no
-) The Rydberg constant revers to the fact that the stock market always goes up over time, i.e. don't worry about your retirement as "Rydberg" told us already 1895. Yes/no
-) Why is the reduced mass required? What is this?

Chapter 13 – Schroedinger eq.

Class 4 continued – Physics primer about Boltzmann statistics

-) Write down the Boltzmann distribution function
-) What does the term "degeneracy of states" refer to?
-) Provide an example for the degeneracy of states from classical physics.
-) Consider a system which has only two states. How does the population of these states with temperature using Boltzmann's statistic?

Class 5 – Physics primer about classical waves &
Start with Schrödinger eq.

-) What is the difference between an oscillation and a wave?
-) What is the definition of a wave?
-) What is a wave front?
-) Define the following: frequency, wavelength, wave vector, angular frequency.
-) What is the relationship between frequency and wavelength?
-) Write down a one-dimensional classical wave equation.
-) What happens if you superpose (add) waves together?
-) What is a standing wave?
-) How can you generate a classical standing wave?
-) What is a "boundary" condition?
-) Write down the classical wave equation.
-) Familiarize yourself with complex functions, i.e., read chapter 13.3 in Engel's book.

-) Does a connection of the classical wave equation and the Schrödinger equation exist? If yes, is this a prove of the Schrödinger Eq.?
-) What are stationary states?

-) What is the difference of standing waves in classical mechanics and stationary states in quantum mechanics?
-) Write down the time independent Schrödinger Eq.
-) What have Newton's law and the Schrödinger Eq. in common?

Class 6 – Physics primer about classical waves
Start with Schrödinger eq.

-) Write down the time dependent Schrödinger Eq.?
-) Define all the symbols in the Schrödinger equation?
-) What is Born's interpretation of a wave function?
-) What is the square root of minus one?
-) What is a nabla operator?
-) What is a complex conjugate?
-) Why is the square of the wave function normalized and not the wave function itself?
-) How to calculate the probability to find an electron?
-) Is the square of a complex function a real or complex function?

Class 7 – Separation of variables

-) What is a stationary state? Provide details. Are the electrons at rest in this state?
-) What properties of the wave function are required in order to obtain meaningful solutions?
-) The wave function must be quadratically integrable. What does this mean? Provide an equation. Why is this required?
-) How does the "separation of variables" method work? (Important)
-) Summarize what you know about the Schrödinger Eq. on one page.

Class 7 and 8 – Operators, Eigenvalues, Eigenfunctions

-) What is an operator? Provide a definition.
-) How is the commutator operator defined?
-) What operator arithmetic rules do you know?
-) How to calculate the square of an operator?
-) Write down the Hamilton operator.
-) Rewrite the time independent Schrödinger equation using the Hamilton operator.
-) What is an eigenfunction and eigenvalue?
-) Is the 1s state an eigenfunction of the Hamilton operator for the H atom?
-) How can a function be orthogonal?
-) What is "a set of eigenfunctions"?

Chapter 14 – Postulates

Class 8 – Postulates (briefly only)

-) What is the theoretical analog in Q.M. to run an experiment?
-) "God does not play dice" refers apparently to Albert Einstein. What is this all about?

Chapter 15 – Q.M. of simple systems

Class 9 – particle in a 1D box

-) You should know this back and forth!
-) How does the potential look like for the particle-in-a-box problem?
-) What are the classical expectations?
-) Where and how do the quantum mechanical solutions deviate from the classical expectation?
-) What results can we expect if we solve the Schrödinger equation? What do we get out of this in principle? Qualitatively?
-) Write down the Schrödinger equation for a particle inside of the box.
-) What is the wave function outside a box with infinite walls?
-) What energy eigenvalues would you obtain for n approaching infinite?
-) How does the wave function look like for large n?
-) Could one manufacture a box small enough to see these effects?

Class 10 – 2D and 3D boxes

One can never have enough box questions:

- Schrödinger equation for the box system?
- Energy eigenvalues
- Can you discuss the results?
- What is the classical limit?
    - For the energy eigenvalues
    - For the wave functions
- Compare finite box with infinite box
- Where is the quantization coming from?
- When does the tunneling effect come into play?
- Compare 1D and 3D boxes
- Can you manufacture this kind of box?
- How to calculate where the particle is in this kind of box?
- Do you see a degeneracy of states for a 1D box?
- What is the degeneracy of states?
- Do negative quantum numbers make sense?
- Does n = 0 makes sense?
- Is E = 0 possible?
- Do the energies become continue for large quantum numbers?
- The box potential is very simple. Is that actually useful for any real system?

Chapter 16 – Tunneling effect

Class 11 – Tunneling effect

-) Describe the tunneling effect. What is that?
-) Name two examples?
-) Assume a simple box potential such as an inverted particle-in-the box problem:
    --) How does the tunneling probability depend on the mass of the projectile?
    --) How does the tunneling probability depend on the size of the potential barrier?
-) Are chemical reactions with isotopes any different?

Note included in exams:

-) What is the basic idea of a scanning tunneling microscope (STM)?
-) Does the tip of the STM touch the surface? Why? Or, why not?

Chapter 17 – Commutator, uncertainty principle

Class 12 – Stern-Gerlach experiment, 6th postulate, and Heisenberg uncertainty principle

-) Explain briefly three of the six postulates.
-) What does the 6th postulate describe?
-) What is a "Commutator"?
-) How is an experiment described in quantum mechanics? (In formal/abstract terms.)
-) Space quantization is a "concept" in Star Trek movies which does not exist in quantum mechanics. Yes/No?
-) What experiment does show that the magnetic moment is quantized?
-) $\left[\hat{x}, \hat{p}_x\right] f\left(x\right) = ?$
-) What is the fundamental limit of experiments? Accuracy / simultaneously availability.
-) Heisenberg came always too late to his quantum mechanics class. Therefore, historian came up with the term "Heisenberg uncertainty". Yes/no?
-) A sheriff stops you in town for speeding at 75 mi/h. You argue with him that he could not determine precisely enough where you were speeding to write you a ticket, since quantum mechanics would clearly state that at a speed of 75 mi/h the position could only be measure with an accuracy no better than 25 mi. Therefore, you were actually out of town where 75 mi/h are perfectly o.k. Any comment? Correct/true/? Why? (I will not bail you out if you try this.)

Class 13 – Heisenberg uncertainty principle & Harmonic oscillator

-) Use a simple thought experiment to show that high precision measurements of a particle's coordinate lead to a large uncertainty for its momentum.
-) What is a wave packet? For what is that model used in quantum mechanics?
-) Apply the Heisenberg principle to a macroscopic object.
-) Can Charles Tucker the IIIrd build a neutron microscope to image electrons?
-) Why does $E_{tot} = 0$ violated the Heisenberg principle?
-) Why is a tunneling effect impossible in classical mechanics?
Consider the classical harmonic oscillator.

Chapter 18 – Vibration & rotations & harmonic oscillator

Class 14 and class 15 – Harmonic oscillator (vibrations)

-) Why is the harmonic oscillator model important, i.e., what are the applications?
-) Summarize the model of the classical harmonic oscillator. (Engel's book chapter 18.6)
-) The energy spacing of the harmonic oscillator increases with increasing quantum number. Yes/No?
-) The Q.M. harmonic oscillator shows the tunneling effect. Yes/No?
-) What is the zero point energy of the Q.M. harmonic oscillator?
-) The wave functions of the Q.M. harmonic oscillator are the so-called Hermite polynoms.
-) The Q.M. harmonic oscillator has quantized energy eigenvalues. Yes/No?
-) Again: what is actually an Eigenvalue?
-) How to calculate the force constant of Q.M. harmonic oscillator if the vibrational frequency is known?
-) What is the equation for the frequency of the Q.M. harmonic oscillator?
-) What would you need to do in order to prove that the wave functions of the Q.M. harmonic oscillator are orthogonal?
-) What would you need to do in order to prove that the wave functions of the Q.M. harmonic oscillator are normalized?
-) What is it important that the wave functions of the Q.M. harmonic oscillator are normalized?
-) What would you need to do in order to prove that a given wave function describes indeed correctly the Q.M. harmonic oscillator?

Class 16 – rotations

-) How does the separation of variables technique work?
-) If the Hamiltonian of a system can be written as $H = H_1 + H_2 + H_3$ who does the total wave function look like?
-) If the Hamiltonian of a system can be written as $H = H_1 + H_2 + H_3$ who does the total energy look like?
-) How can the Hamiltonian of a rigid and two atomic molecule be written?
-) What are the energy eigenvalues of the rigid rotor?
-) What is the correlation of the energy eigenvalues and the angular momentum of the rigid rotor?
-) Write down the eigenvalue equation of the angular momentum for a rigid rotor.

Class 17 – 3D rigid rotor

-) Write down the structure of the wave function for the 3D harmonic oscillator. In what functions does the wave function separate? On what coordinates do these functions depend? What quantum numbers are involved?
-) What quantum numbers are included in the description of the 3D harmonic oscillator?
-) Compare the energy eigenvalues of the particle-in-a-box, the harmonic oscillator, and the rigid rotor?
-) Has the rigid rotor a zero point energy? Yes/No (Explain)
-) What is the degeneracy of states concept?
-) Compare the degeneracy of states for the 3D particle in a box and 3D rigid rotor.
-) Explain the equation $\hat{l}_z\Phi(\phi) = \pm m_l h\Phi(\phi)$

in your own words. Hint: Let's assume one would like to measure the z-component of the angular momentum of the rigid rotor. How to do that in formal Q.M. terms? What would be the result? Remember this formalism from the Stern-Gerlach experiments.

Class 18 – start with spectroscopy, Einstein coefficients, Fermi's golden rule, and selection rules

-) How would you define spectroscopy in one sentence?
-) What do we learn if we apply spectroscopic techniques to a given system?
-) In what range of the electromagnetic spectrum are rotations and vibrations of molecules?
-) Einstein came up with coefficients to predict accurately his retirement, today they are just called Einstein coefficient to indicate that he was always very efficient. Correct? Yes/No.
-) Explain the term stimulated adsorption, stimulated emission, absorption.
-) What is Fermie's golden rule? Write it down & explain.
-) What is a selection rule in quantum mechanics?
-) What are the selection rules for micro wave spectroscopy or pure vibrational spectroscopy?
-) How to prove the selection rule for the 1D particle-in-a-box problem?

Chapter 19 – Vibrations & rotations & Raman spectroscopy (applications)

Class 19 – vibrations and absorption spectroscopy

-) How do the selection rules for the harmonic oscillator look like?
-) Define what a selection rule is.
-) Define absorption spectroscopy
-) What is the Lambert-Beer law?
-) Name current applications (i.e. interesting systems) for absorption spectroscopy.
-) What leads to greater vibrational frequencies double or single bonds?
-) How does the stretching vibrations wavenumber shifts when deutorating a single bond? C-H vs. C-D?
-) What is deuterium?

Class 20 – pure rotation spectra, rotation and vibration spectra

-) What are the selection rules for the particle-in-a box, harmonic oscillator, rigid rotor?
-) What are typical energies for rotations and vibrations?
-) What type of interaction do we consider? Magnetic? Electric?
-) What are the energy eigenvalues for rotations in quantum mechanics?
-) Calculate a rotational spectra, i.e., how large is the energy spacing between adjacent rotational levels?
-) What is a wavenumber?
-) How large is the degeneracy of states for rotations? Is that important for something?
-) The R and P branches are a special office at US bank for private and business customers. Correct/wrong?
-) Why is a gap in rotational spectra?
-) Explain the intensity variations seen in rotational & vibrational spectra.
-) Why can different definitions for the rotational constant be found in the literature?
-) What is a pure rotation spectra and how could you get one?

Class 21 – rot/vib spectra continued - FTIR

-) What is an R and P branch in IR spectra?
-) What is the main concept of FT-IR?
-) What is a Fourier transformation?
-) What is a dispersion type IR system? Compare with FT IR.
-) What is the advantage of FT IR?
-) How to calculate the bond length from rot/vib spectroscopic data?
-) What is HREELS? (Supplemental question.)
-) How does deuterating a molecule affect the vib/rot spectra?
-) What is the basic idea of a Michelson interferometer?

Class 22 – Raman spectroscopy

-) What is a stokes shift?
-) What are stoke and anti-Stockes lines?
-) Who is Raman? New low fat sandwich makings?
-) What is the origin of Raman lines? What is the basic mechanism?
-) Compare the selection rules for Raman an IR spectroscopy?
-) Raman line positions shift with variations of the excitation frequency. Yes/No? Why?
-) Write down the energy conservation law for Raman spectroscopy.
-) What Raman lines have greater intensity Stokes or anti-Stokes lines?
-) What is a Rayleigh line in a Raman spectrum?
-) Write down an expression for the time dependent polarization of a molecule.
-) Did you look at the "self-tests" discussed in class?

Chapter 20 – Hydrogen atom

Class 23 & 24 & 25 – Hydrogen atom

-) What is a Coulomb potential?
-) Write the Hamiltonian for H atom in Cartesian coordinates.
-) Outline the basic ideas of the solution of the H atoms in Q.M.
-) Why are the solutions for the rigid rotor and the angular components of the H atom identical?
-) In what functions does the wave function separate?
-) What is a radial function?
-) Why are linear combinations of the wave function used?
-) What are the relevant quantum numbers?
-) What are the energy eigenvalues?
-) What is the degeneracy of states?
-) Name strategies to visualize the wave functions of the H atom.
-) Radial distribution function plots
-) Why is the radial distribution function rather than the square of the magnitude of the wave function used to make a comparison with the Bohr atom model?
-) If the probability density of finding the electron in the 1s orbital in the H atom has its maximum value for r = 0, does this inquire that the proton and electron are at the same point in space?
-) Is the z direction special?

Class 26 – Electron spin

-) What experiment provides an experimental verification of the electron spin and why?
-) Compare the relevant equations for the orbital momentum and the electron spin.
-) What is the spin orientation quantum number?
-) How do spin orbitals look like?
-) What are the eigenvalue equations for the angular orbital momentum and the spin angular momentum?

Class 27 – Pauli principle

-) Write down two versions of the Pauli principle.
-) What is the symmetry of the complete wave function?
-) What is a Slater determinant?
-) What is an exchange interaction?

Chapter 21 & 22 – Many-Electron Atoms

Class 28 – Variation principle and Hartee Fock

-) What is the variation theorem?
-) What is the basic idea of the HF technique?

Class 29 – Singlet / triplet states

-) What is the vector model for singlet and triplet states?
-) What are the relevant operators for single and multi electron systems?
-) What are good and bad quantum numbers?

Class 30 – Term symbols

-) What are equivalent and non equivalent electrons?
-) What is a subshell?
-) what is the idea of procedures to derive the term symbols from the electron convigurations?
-) One may want to look at numerous examples.
-) Why are term symbols used?

Class 31 – Hund's rules

-) What and Hund's rules 1^{st}, 2^{nd}, 3^{rd}…
-) What is the purpose of those rules?
-) What is a spin orbit coupling?
-) Why is the quantum number "j" intdroduced?
-) What happens with a sample in an external magnetic field?
-) What is the difference of the Zeemann effect and the spin orbit coupling?

Class 32 – Born Oppenheimer Approximation

-) What is that? Explain.
-) Why is this typically a good approximation?
-) How is the mathematical procedure called used to treat the different components to the Schrödinger equation separately?

Class 32 – Born Oppenheimer Approximation

-) LCAO is what?
-) Write down the wave function for H2+.
-) What is an overlap integral?
-) What is the difference between a bonding and antibonding wave function?
-) What is a simple classical interpretation of the overlap integral?
-) Explain MO, AO?

Class 33 – MO theory, examples

-) Draw a MO diagram and explain how to read it.
-) Pi, sigma, *: explain.
-) g, u: explain.
-) What is a bond order? Why is this concept useful?
-) Is He2 stable?
-) What is the electron configuration of NCl? What is the bond order?
-) Why is the ionization energy of CO greater than the one of NO?

Exam preparation guide

No, this is not an immigration form for a green card application but it reminds me a little on it. If you answer one of the following questions with **no** you may run into **problems** with your next exam:

	Check the appropriate box.	
	Yes	*No*
Do you write an own summary of the class?	☐	☐
Do you read the textbook?	☐	☐
Do you look through the homeworks before the exam (in detail)?	☐	☐
Do you read your class summary before the exam?	☐	☐
Do you study carefully the examples discussed in class?	☐	☐
Do you look for typos (wrong sign +/-) in class room examples?	☐	☐
Have you memorized the most important equations of your own summary draft?	☐	☐
Have you checked your draft for typos?	☐	☐
Do you memorize and understand concepts?	☐	☐
Do you plan to sleep at least 8 hours before the exam?	☐	☐
Do you plan to start the exam preparation at least one week before the exam?	☐	☐
Do you work together with your class mates?	☐	☐
Looked at study guide?	☐	☐
Studied old quizzes?	☐	☐

By the way:
We all tend to study what we already know.
But – this does not really help.
Focus on topics you could not understand so well, so far.
Look it up again and/or ask.