CHE502

A few concepts you should master and things you should know without consulting a book or the Internet not necessarily in the order in which they were taught

to encourage your lateral thinking

some answers you probably also know from previous classes. Put them into context

- 1. What is roughly the length of a typical O-H (or C-H or ...) bond in a molecule?
- 2. Which experiments demonstrated (in the 1920ies) that in certain cases classical (Newton's) mechanics was not a suitable description?
- 3. Describe the Hamiltonians \hat{H} for a few one-dimensional (model) problems
- 4. Which theory endeavors to link the microscopic description of matter with macroscopic observable?
- 5. Why would you prefer a linear fit (if possible) to a non-linear one?
- 6. What is a quantum mechanical 'state'?
- 7. What are (pseudo-) random numbers? What are they good for?
- 8. How are classical mechanics and quantum mechanics related?
- 9. What is the zero-point energy (ZPE)?
- 10. Sketch the wavefunction $\psi_1(r)$ for the ground state of the hydrogen atom H and the He⁺ ion. Are they the same or are they different? Why?
- 11. Explain the concept of 'equal a-priori probability' in statistical mechanics
- 12. Molecules can store and exchange energy in various ways. However, the magnitudes of the energy quanta involved are different. List some of these possibilities and rank them by the magnitude of the quanta
- 13. What is 'phase space'?
- 14. What is the relation between the frequency of a radiation and the energy of a quantum of this radiation?
- 15. List in order of increasing energy the domains of the electromagnetic radiation and with which
- 16. What are the conditions for a molecule to absorb a quantum of electromagnetic radiation?
- 17. What is a Boltzmann factor? What does it tell you?

- 18. What is degeneracy / degenerate states?
- 19. What are typical distances between 'small' molecules (H₂O, CCl₄, CH₃OH and such) in their liquid phase?
- 20. What is the characteristic difference between 'scattering' (eg. X-ray scattering) and 'spectroscopy' (eg. Infrared)
- 21. What is the relation between the wavelength and frequency of an electromagnetic radiation?
- 22. Can equilibrium constants (of gas phase reactions) be computed from the partition functions of the molecules?
- 23. How does the zero point energy (ZPE) depend on the mass of the particle involved?
- 24. I put N molecules of something into a fixed volume V. How can I fix the temperature T and the pressure p at desired values and still keep the system in one homogeneous phase?
- 25. X-rays are electromagnetic radiation. When I do X-ray scattering, with which particles does the radiation interact?
- 26. and more