

Chemistry 276 - Autumn 2009-10 - Advanced Physical Chemistry

Final Paper

Choice of topic. Pick a topic that is of interest to you and that is consistent with the following guidelines.

- It should be directly related to one or more of the main topics of the course:
 - the use of equilibrium correlation functions to describe
 - * relaxation processes
 - * scattering experiments
 - * spectroscopic experiments
 - the various types of dynamics used to explain these correlation functions
 - * classical mechanics
 - * Langevin dynamics and related stochastic dynamics (random walks, Brownian dynamics, Monte Carlo)
 - * quantum mechanics
 - * collision models
- It should be something that you are interested in (perhaps related to your research) but that you don't already understand in detail.
- It is small enough that the important issues of concern to you can be discussed in a short paper.

One possibility would be to pick a specific relaxation process, scattering experiment, or spectroscopic experiment that can be related to correlation functions (e.g. nuclear spin relaxation in NMR, or viscosity and viscoelasticity of polymer solutions, or Rayleigh light scattering from fluids, or TG-OKE measurements of rotational relaxation) and discuss how correlation function formulas are derived and how they are related to experimental observables. (Perhaps also discuss the uncertainties and assumptions in the derivations and the effect this has on the interpretation of the experiment.) You don't

have to limit yourself to linear experiments. Nonlinear experiments are ok as topics. Another possibility would be to pick a specific physical problem and discuss two different associated measurements and the relationship between them (e.g. the structure of liquid water as determined from x-ray scattering and neutron scattering, or rotational motion of molecules as measured by Rayleigh scattering and Raman scattering). A third possibility would be to pick two types of dynamics and discuss how they are related theoretically (e.g. classical mechanics and Brownian dynamics, or Langevin dynamics and Smoluchowski dynamics). I would be open to any suggestions you might have even if they don't appear to fit into any of these categories.

Instructions. The paper should be brief (five typed pages of text, plus bibliography and, if needed, figures).

The actual writing of the paper will be the minor part of the work. The purpose of this assignment is to give you the opportunity to study, in some detail, some aspect of the course subject that is of interest to you.

The paper should demonstrate that you have in fact learned something from your study. It should not simply be a summary of published material. You should make connections with the discussion in lecture or homework, evaluate assumptions critically, compare contrasting theoretical or experimental methods in some useful way, carry out some detailed derivation that is swept under the rug in the usual papers, investigate something you don't understand so that you either do understand it or identify clearly the problematic issues, or something along these lines. Then write a paper that makes it clear that you have learned something and exercised your own judgment and/or performed your own independent analysis. (You can go over the page limit if necessary, but don't take this as an invitation to write a massive paper.)

Write the paper as if the reader were another graduate student in the course, who understands what correlation functions are but who does not know much about your topic. Imagine that you are preparing to give a lecture to the class on your topic. Figure out what would be most important points to discuss in detail and what theoretical derivations would be useful.

The topic could be quite narrow (narrower than many of the suggestions I have seen in previous years) and/or quite elementary (more basic than some of the suggestions I have seen in previous years), as long as you thoroughly

investigate the topic, use your own judgment, and write a paper showing that you have learned something.

Please make the paper clear and readable. If you can convert the final paper to a .pdf file, then send it to me as an e-mail attachment (to hca@stanford.edu). Otherwise, put a hard copy in my mailbox in the main chemistry office before the deadline. When you turn in your paper, attach copies of any literature papers that you have relied on extensively (a pdf version electronically submitted is preferred, but paper copies into my mailbox are ok).

If you have any questions, don't hesitate to contact me. E-mail is the most effective way of doing this.

Schedule

- Friday Nov. 20, 11:00 pm: Preliminary proposal for paper topic is due. (Send to hca@stanford.edu.) Briefly describe the topic and the literature materials you will focus on.
- Monday Nov. 23, 5:00 pm: By this time I will respond to your proposal, either approving it or making suggestions for alternatives.
- Wednesday Nov. 25, 5:00 pm: If I did not approve your proposal the first time around, your revised proposal is due at this time.
- Friday Dec. 4, 11pm : Paper is due (preferably in pdf form sent to hca@stanford.edu with copies of papers you relied on, or hard copies in my mailbox in the main Chemistry Department office).