Chemistry 532
Advanced Physical Chemistry II
Course Syllabus
Fall 2012

1. Instructor: David L. Freeman
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   Office: 333 Pastore
   Office Hours: MWF 10, or anytime.

2. Scheduling: TuTh 11:00 AM - 12:15 PM, 219 Pastore

3. Text: *Quantum Chemistry* by Donald A. McQuarrie, University Science Books.

4. Prerequisites: CHM 432 or permission of instructor.

5. Course requirements:

a	Two one hour exams at 100 points each	200
b	Homework	50
c	Final exam	200
d	Total	450

   The exams will be primarily problems with some definitions. Grades will be determined on a curve with B as the average. All exams will be closed book. Incompletes will be given only for valid medical reasons.

6. Course goals:

   Those of you who have taken Chemistry 531 have learned the method chemists use to systematize and rationalize macroscopic phenomena. The laws of thermodynamics form the appropriate organizational tool to understand the chemistry of bulk systems.

The laws of thermodynamics fail to give any microscopic description of chemical systems. In statistical mechanics we do explain chemical and physical properties and dynamics in the thermodynamic limit from a knowledge of the microscopic properties of the constituent atoms and molecules of a bulk system. To complete the connection, we need to know the microscopic laws explicitly. The laws of non-relativistic quantum mechanics, which provide a complete description of chemistry at the microscopic level, form the basis for our studies this semester.

Most of you have had an introduction to quantum mechanics in your junior level physical chemistry courses in college. At the graduate level we will study quantum theory in more depth. A prerequisite to an appreciation of quantum mechanics is knowledge of some areas of mathematics which many of you may not have learned as undergraduates. Examples of some of these areas of mathematics are differential equations and Fourier transform methods. Because this mathematics is unfamiliar to many of you, our first course goal is *to learn the mathematics necessary for the study of quantum theory.* Our emphasis will be on applied rather than formal mathematics.

Once the necessary mathematics has been presented, we can turn our attention to physical phenomena. As we shall learn, the behavior of electrons is governed by equations which are analogous to the equations of classical wave motion. Thus our second course goal is *to learn the properties of classical waves.* With this background in classical wave motion, we will be prepared *to learn the experimental basis of quantum theory*, which is our third course goal.

With the necessary experimental background, our task will be to construct the correct theory for microscopic phenomena. This theory is embodied in the Scrödinger equation. Our fourth course goal will be *to learn the Scrödinger equation and its applications to elementary chemical problems.*

It is to be emphasized that the discovery of the Scrödinger equation was one of the major intellectual achievements of the twentieth century. Its philosophical implications have been extensive. Our final course goal is *to understand the historical and philosophical implications of quantum theory.*

7. The CHM 532 Web page:

   In this course all handouts, problem sets, problem set solutions and exam solutions are to be distributed on the course web page. No paper copies of the solutions are to be distributed. The URL of our course web page is
   http://www.chm.uri.edu/courses/?chm532&1 . It is strongly suggested that you link to our web page as soon as possible.

   It is expected that for most of you, success in this course will require some level of help beyond classroom instruction. Because some of you work off the main campus and may find it difficult to come to the scheduled office hours, we have installed as part of our course web pages, a page that can be used to submit questions. Questions are submitted by anyone in the class by filling out a form on the web page, and answers are distributed either to the entire class or only to the person asking the question. If the entire class is to receive a copy of the question and answer, the question is treated as anonymous; i.e. the person who asks the question is never identified. In fact, it is possible to submit a question so that even the instructor does not know who submitted the question. Anonymous questions and responses by the instructor are distributed automatically to everyone who has submitted their e-mail address to the instructor. With ordinary electronic mail, there is a private correspondence between the student and instructor. By using the web page, the entire class has an opportunity to learn from the questions submitted.

The use of the web page does not preclude personal interaction between any of you and the course instructor. My office is always open to graduate students, and you are all encouraged to come to my office for help. Additionally, you can contact me by e-mail or telephone. My e-mail address and phone number are given on the first page of this syllabus.

To receive copies of the submitted questions and the answers to the questions, you must submit your e-mail address. To submit your address, go to our home page (http://www.chm.uri.edu/courses/?chm532&1) and click on "Subscribe to the CHM 532 list." On the resulting form, enter your e-mail address, click on the small "subscribe" button and then click on the submit button. You can also use this form to unsubscribe from the list in case you drop CHM 532.

Any student in CHM 532 can submit questions and comments to me. Submission of such comments or questions must be made using the WWW home page for this course. The address (URL) of our home page is
http://www.chm.uri.edu/courses/?chm532&1 . To submit a question to the list, you must click on the highlighted text that says "submit a question to the CHM 532 list."

As an example of how to use the list, suppose a student in our class, Ms. Benzene Ring, wonders, "What are the units of wavefunctions?" (If you don't know what this means, don't worry. You will understand the question during the semester). To obtain an answer to her question, Ms. Ring links her web browser (e.g. Firefox, Safari or Internet Explorer) to http://www.chm.uri.edu/courses/?chm532&1, and she then clicks on the text linking her to the page for questions (i.e. the highlighted text that says "submit a question to the CHM 532 list"). Ms. Ring then enters (optionally) her e-mail address in the appropriate box and specifies whether she wants her question to be answered to the entire CHM 532 list or to her alone. Ms. Ring then types in the large box

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What are the units of wavefunctions?
```

Ms. Ring then clicks the "send" button. Ms. Ring's question is received by me. I then send an e-mail message to the whole list that might be

```
Subject:  wavefunction units
The question is:  What are the units of wavefunctions?
```

`Answer: In one dimension, the units are 1/\sqrt{length}. In three dimensions the units are 1/\sqrt{volume}.`

Now Ms. Ring and the entire class have an answer to her question. In the answer `\sqrt{}` stands for a square root, and this notation is discussed below.

If the answer to the question can be sent to the entire list, the answer will not indicate who asked the question. If Ms Ring wants to ask the question with full anonymity so that even I have no idea who asked the question, the e-mail portion of the form can be left blank. Of course, if the e-mail section of the form is blank, the answer must be sent to the list and not just to the sender.

Because many questions may contain mathematical formulas, we need a notation to communicate the special symbols used in the course. To avoid confusion, it is most useful if we agree on the same set of symbols. The symbols that follow are taken from a language called LaTeX. LaTeX is a language that is frequently used to prepare scientific documents, and LaTeX can be used to translate special symbols into simple text characters. By learning LaTeX notation, you will learn a widely used method to communicate mathematical symbols via e-mail. The instructor plans to use these symbols in answering your questions, and it is asked that you use the same symbols in posing questions. The most important symbols are the following:

(a) Greek letters are represented by \ followed by the name of the letter. For example α is typed `\alpha`, β is typed `\beta`, and so on. A Greek letter is made upper case by making the first letter of its name upper case. For example, the letter Δ is typed `\Delta`.

(b) Subscripts are represented by `_{}` where the brackets contain the subscripts. For example, μ_{ij} is typed `\mu_{ij}`.

(c) Superscripts are represented by `^{}` where the brackets contain the superscripts. For example, β^{12} is typed `\beta^{12}`.

(d) Infinity (∞), is typed `\infty`.

(e) The integral sign $\int$ is typed `\int`. The limits on a definite integral are included by introducing subscripts and superscripts. As an example $\int_0^\infty e^{-x^2} dx$ is typed `\int_{0}^{\infty} e^{-x^{2}} dx`.

(f) The partial derivative symbol ∂ is typed `\partial`.

(g) The summation sign $\sum$ is typed `\sum`. The lower and upper limits of summation are included as subscripts and superscripts. As an example $\sum_{n=0}^\infty 1/n^2$ is typed `\sum_{n=0}^{\infty} 1/n^{2}`.

(h) Square roots $\sqrt{a+b}$ are typed `\sqrt{a+b}`.

(i) The arrow in chemical reactions $\rightarrow$ is typed `--->`. For example $C+O_2 \rightarrow CO_2$ is typed `C + O_{2} ---> CO_{2}`.

Let us now look at another example of a question submitted using the web. In this case, Ms. Ring has a question requiring an equation. This might be a real question. If you don't understand the context, don't worry. You will understand the details of the question later in the course. Suppose Ms. Ring wants to ask

"In calculating an expectation value, the expression is

$$\langle A \rangle = \int_{-\infty}^{\infty} \psi^* \hat{A} \psi dx$$

For calculating the expectation value of the momentum, what operator do we use for A?"

To submit the question, Ms. Ring uses her web browser to attach to http://www.chm.uri.edu/courses/?chm532&1, clicks on the line that says, "submit a question to the CHM 532 list," and then Ms. Ring enters the information requested by the form. If Ms. Ring wishes to remain anonymous, Ms. Ring leaves the e-mail box blank. Ms. Ring then types into the large box

```
In calculating an expectation value, the expression is
< A > = \int_{-\infty}^{\infty} \psi^* A \ psi dx For calculating the expectation
value of the momentum, what operator do we use for A?
```

and clicks on the submit button. Ms. Ring's question is received by me. The answer will be sent either to Ms. Ring alone, or preferably to the entire class if the appropriate box is checked. I might reply

```
Subject:  Momentum Operator
The question is:In calculating an expectation value, the expression is
< A > = \int_{-\infty}^{\infty} \psi^* A \ psi dx For calculating the expectation
value of the momentum, what operator do we use for A?

The answer is:  A=p=hbar/i d/dx
```

Remember, your first task is to subscribe to the CHM 532 list either by e-mail or filling out the form on our web pages. You can then send questions and comments to me using your web browser starting at the URL
http://www.chm.uri.edu/courses/?chm532&1

8. Course Outline

Topic	Reading Assignment
1. Review of Calculus	Text, Section 2.3
2. Historical Introduction	Text, Chapter 1
3. Classical Mechanics	Handout

4. Classical Wave Motion	Text, Chapter 2
5. Fourier Series, Fourier Transforms and the Delta Function	Handout
6. The Experimental Basis of Quantum Theory	
7. Vectors	
8. The Schrödinger Equations and the Particle in a Box	Chapter 3
9. Exam Number 1	
10. Operators and the Theorems of Quantum Mechanics	Chapter 4
11. The Harmonic Oscillator	Chapter 5
12. Angular Momentum	Section 6.7
13. Exam Number 2	
14. Three-dimensional Systems and the Hydrogen Atom	Chapter 6
15. The Variational Theorem	Chapter 7
16. Final Examination Thursday, December 20, 11:30-2:30	Comprehensive