Problem Set 2

Physical Chemistry I
Fall 2005
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This problem set is due in class on Friday, September 9. Read Chapter 3 sections 3 to 9 and complete the selection of problems below.

Problems from McQuarrie and Simon You may (and are in fact *encouraged*) to work with other members of the class on these problems. Solutions can be found on reserve in the Collier Science Library, but you should only consult these to check your work or *in extremis*.

Math Section A: A-5
Chapter 3: 1, 2, 3, 5, 9

Test Yourself When completing the problem below, you may not consult anyone. You may use the text and notes and problems sets written in your own hand. If you use Mathematica, please print out the notebook and attach it.

Two operators are said to commute if

$$\hat{A}\hat{B}f(x) - \hat{B}\hat{A}f(x) = 0$$

In fact, you can define an operator, called the commutator that has the form

$$\hat{A}\hat{B} - \hat{B}\hat{A}$$

Many operators do not commute, and their commutator is itself a non-zero operator that changes the form of one function to another. Find the commutator operator for

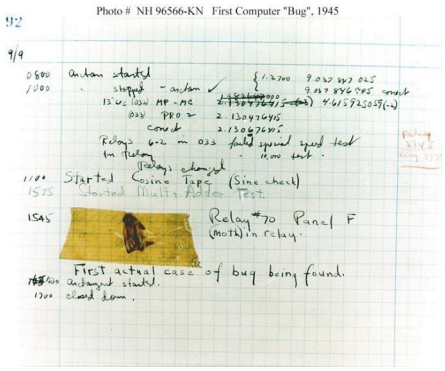
$$\hat{A} = \frac{d^2}{dx^2}$$

$$\hat{B} = x\times$$

by finding $\hat{C}$ below.

$$\hat{A}\hat{B}f(x) - \hat{B}\hat{A}f(x) = \hat{C}f(x)$$

The Culture of Chemistry



The solution of differential equations has taken on an entirely new dimension in the 75+ years since Schrodinger proposed approaching the description of matter waves using PDEs. The solution of many differential equations can now be found numerically, using computers. Grace Hopper, who graduated with a BA in math from Vassar, a women's college, in 1928. She worked on her doctorate in math at Yale and returned to Vassar as a professor of mathematics in 1931. During WW II she joined the waves and was assigned to the team running the Mark I - an early digital computer. Her work there eventually led her to design the first compiler - a translator which turns the "natural" language of the programmer into the binary code that the computer can read. Hopper hoped that then "the programmer may return to being a mathematician." The development of widely used symbolic algebra programs such Mathematica and Maple can be traced to Grace Hopper's work. Legend has it that Grace Hopper is the one who coined the term "bug" for problems with a computer, after pulling a moth out of one of the machines.