Problems

Problems marked with * are meant to be solved without the aid of a computer.

(1) * Using the Taylor's series expansion for

$$f(x_0 - 2h), \quad f(x_0 - h), \quad f(x_0 + h), \quad \text{and } f(x_0 + 2h)$$

derive a five point formula for the first derivative with an error proportional to $h^4 f^V(x_0)$. The central point will not appear in the formula. Hint: consider the expressions for $f(x_0 + 2h) - f(x_0 - 2h)$ and $f(x_0 + h) - f(x_0 - h)$.

(2) Use the program "diff" to compare with Table 25.2 in Ref. I for 3, 4 and 5 points for the first and second derivatives.

(3) Use the method described in the text and Eq. 3.28 to solve for $rj_\ell(kr)$ for $\ell = 0, 1, 2, 3$, and 4. Take the ratio to the exact functions calculated with the use of the function SJ (see Appendix A.3). Discuss the behavior of this ratio for the different values of ℓ. In what way are the functions for $\ell = 3$ and 4 different.

(4) Release the piston in the molecular problem described in the text by making the mass ratio only [illegible]:1. Follow the cooling of the gas and the energy of the piston.

(5) Generalize the molecular problem to allow the molecules to have an excited state. Define a vector `is(i)` to distinguish the state of the molecules, `is=0` meaning that the molecule is in its ground state and `is=1` that it is in its first excited state. Assume that the energy of the excited state is, E^*, is 0.1 eV. When a collision occurs assume that with probability

- $\frac{1}{4}$ neither molecule changes its state
- $\frac{1}{4}$ molecule 1 changes its state
- $\frac{1}{4}$ molecule 2 changes its state
- $\frac{1}{4}$ both molecules change their state.

If the center-of-mass energy is insufficient for the branch chosen, try again by choosing the probabilities. A simple way to implement the four choices above is to generate a uniformly distributed random number between 0 and 1, multiply it by 4 and add 1. Fix the result and take the four branches according to the value of the variable.

a) Start all of the molecules in their ground state and follow the population distribution of the excited states.

b) Assume that at the 10^{th} time step a laser is flashed through the cylinder putting all of the molecules in the excited state. Follow the temperature evolution of the gas.

(6) * Suppose that you wished to generalize the molecular collisions in the simulation in this chapter to be non-isotropic. If the scattering cross section is proportional to the square of the cosine of the angle between the initial and final center-of-mass momenta describe one way to implement such a distribution in a practical case.

Chapter 4

Computers for Physicists

The development of the modern computer was greatly influenced by the ideas of von Neumann, Burks and Goldstine in 1946 which outlined much of the logical constitution of the systems we know today. Of course, these ideas themselves were built on many previous advances. One of these of great importance was due to Hollerith who, trying to solve the practical problem of tabulating the census of 1880, introduced the use of punched cards in 1886 to enter information into a computing engine. This work was, in turn, based on a mechanical use of punched cards to drive weaving machines invented by Joseph-Marie Jacquard in France in the early 1880's. Much of the present-day logic is based on Boole's *Treatise on Differential Equations* (1859). It is not clear what role (if any) the work of Charles Babbage in 1835 had on the development of the computing devices we see today. It appears that he was too far ahead of his time.

Thus, Von Neumann's step was, in some sense, a remarkable one but based on a good deal of previous work. At the time of this contribution the second world war had just ended and work on the Manhattan project had shown that high speed computing was the key to designing weapons and perhaps many other things. The computation available at the time operated with "plug-boards" which determined the route the numbers would take in the interior of the machine. If one wanted to change a program it was necessary to remove the board and re-wire it. The suggestion made in the von Neumann work was to allow the instructions which route the data to reside in memory also such that the control of data flow would be subject to alteration by the program. Babbage had already designed such functions into his machine more than a century earlier.

In fact, it is now rare that one modifies the program in the middle of a calculation (modern compilers either discourage or prohibit it, with good reason) but instead what has resulted are compilers, assemblers and other logic manipulators which create instructions from higher level input.

The major defining characteristic of a computer is its ability to do large calculations rapidly. This rapidity is measured in terms of its "clock period". The "clock", as it is often called, is the time for a basic operation to be performed, that is, for the simplest instruction to be executed. This fundamental time has been a defining parameter of computers since the time of Hollerith when a rotating drum delivered the punched cards to the machine at a fixed rate. At the present time it is more common to hear the speed quoted as the inverse of the clock period or as a frequency.

In this chapter the architecture of several modern computers is discussed to