Name: PHY401 (Fall 2005), 10/21/05

Homework Assignment #6

(*Due Date*: Wednesday, November 02, 12:40 pm, in class)

6.1 *3-D Random Walk* (cf. Exercise 7.2 in the textbook) *(3 pts.)*
Write a FORTRAN program to simulate a random walker in 3 dimensions, taking steps of unit length but of arbitrary direction (i.e., do not restrict the walker to discrete lattice sites). Show that the motion is diffusive with $\langle r^2 \rangle \propto t$ and determine the value of the proportionality constant.

6.2 *Diffusion Equation* (cf. Exercise 7.9 in the textbook) *(3 pts.)*
Write a FORTRAN program to solve the 1-D diffusion equation using the finite difference form with diffusion constant D=2. Start from an initial density profile (e.g., box profile) that is sharply peaked around x=0 but extends over at least several grid sites. Show that at later times the numerically calculated density profile corresponds to a normal distribution with $\sigma = \sqrt{2Dt}$.

6.3 *Diffusion and Entropy* (cf. Exercise 7.12 in the textbook) *(4 pts.)*
Consider a 2-dimensional distribution of 400 test particles (immersed in a liquid, e.g.) which are initially localized uniformly within a 10×10 square in the center of a 200×200 boundary (as in Section 7.5 of the textbook). Simulate its diffusion process by randomly choosing one particle per time step and moving it randomly one unit in $\pm x$ or $\pm y$ direction. Calculate the time evolution of the single-particle entropy by evaluating (and plotting)

$$S_1 = -\sum_i P_i \ln P_i \ , \tag{1}$$

using all 400 particles to determine the probability P_i for finding one particle within a site of a 8×8 partition of the entire square, at each time step. Confirm, in particular, the asymptotic (equilibrium) value of $S_1(t \to \infty) \sim 4.2$.