Name: PHY401 (Spring 2010), 04/09/10

# Homework Assignment #8

(*Due Date*: Monday, April 19, 10:20 am, in class)

8.1 *Diffusion Equation* (cf. Exercise 7.9 in the textbook) *(1+3 pts.)*

(a) Show analytically that the spatial expectation value, $\langle x(t)^2 \rangle$, of the 1D Normal Distribution,

$$\rho(x,t) = \frac{1}{\sqrt{2\pi\sigma(t)}} \exp[-\frac{x^2}{2\sigma(t)^2}] , \tag{1}$$

equals $\sigma(t)^2$.

(b) Write a FORTRAN program to solve the 1D diffusion equation using the finite difference form with diffusion constant $D$=2. Start from an initial density profile that is sharply peaked around $x$=0 but extends over a few grid sites (box profile). Verify (using a fit) that at later times the numerically calculated density profile corresponds to a Normal Distribution with $\sigma = \sqrt{2Dt}$ (i.e., perform a fit for 5 different time snapshots over which significant changes of the distribution are visible).

8.2 *Diffusion and Entropy* (cf. Exercise 7.12 in the textbook) *(3+3 pts.)*

Consider a 2D distribution of 1000 test particles (e.g., a drop immersed in a liquid) which are initially localized uniformly within a 10×10 square in the center of a 300×300 boundary (similar to Section 7.5 in the textbook).

(a) Write a FORTRAN code to simulate the diffusion process of this "drop" by randomly choosing one particle per time step and moving it randomly by one unit in either $\pm x$ or $\pm y$ direction. Display time snapshots of the particle distribution when noticeable changes are visible.

(b) Calculate and plot the time evolution of the entropy per particle by evaluating

$$S_1 = -\sum_i P_i \ln P_i , \tag{2}$$

using all 1000 particles to determine the probability $P_i$ for finding one particle within a cell of a 12×12 partition of the entire grid. Calculate analytically the initial and asymptotic values of the entropy per particle ($S_1(t{=}0)$ and $S_1(t{\to}\infty)$, respectively) to check your numerical results.