18.325 Topics in Applied Mathematics, Spring 2001, Prof. Bazant.

Problem Set 1a

Due at lecture on Tu Feb 27. (Problem Set 1b may follow.)

1. Let $c(x,t)$ be the probability density for a random walker (or, equivalently, the concentration of a large number of independent walkers) to be at position x at time t. The walker's displacements $(x,t) \to (x', t+\tau)$ are independently chosen with a non-stationary transition probability $p(x', t+\tau|x,t)$ at regular intervals of time τ. Suppose that the moments

$$M_n(x,t,\tau) = \int p(x+y, t+\tau|x,t) y^n dy \tag{1}$$

are finite, and derive the Kramers-Moyal forward expansion,

$$\frac{\partial c}{\partial t} + \sum_{n=2}^{\infty} \frac{\tau^{n-1}}{n!} \frac{\partial^n c}{\partial t^n} = \sum_{n=1}^{\infty} \left(-\frac{\partial}{\partial x}\right)^n [D_n(x,t,\tau)c(x,t)] \tag{2}$$

where $D_n(x,t,\tau) = M_n(x,t,\tau)/(n! \cdot \tau)$. Assume $D_n(x,t,\tau) \to D_n(x,t)$ for $n \le 2$, and derive the Fokker-Planck equation in the limit $\tau \to 0$.

2. Solve for $c(x,t)$ $(x, t \ge 0)$:

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2}, \quad c(x,0) = c_o, \quad -D\frac{\partial c}{\partial x}(0,t) = J, \quad c(\infty, t) = c_o. \tag{3}$$

for both positive and negative values of J. These solutions represent the concentration profiles at the anode and cathode, respectively, in a galvanostatic (constant current) electrochemical cell. In the case $J < 0$, derive an analytical expression for Sand's time t_s, when the concentration vanishes at the cathode, $c(0, t_s) = 0$, and the current J can no longer be maintained due to diffusion limitation.

3. Consider a symmetric random walk on the integers, i.e. starting from the origin, at each time step $n \ge 1$ the walker has equal probability (1/2) of stepping from m to either $m+1$ or $m-1$. Let M_N be the number of time steps $1 \le n \le N$ that the walker is on one side of the origin (e.g. $m > 0$). Define a scaled cumulative density function for M_N as follows,

$$P_N(\zeta) = \text{Prob.}(M_N \le \zeta N), \tag{4}$$

where $0 \le \zeta \le 1$ is the fraction of time (less than N) the walker spends on one side of the origin. Derive an expression for $P(\zeta) = \lim_{N\to\infty} P_N(\zeta)$. You can try to do this analytically, but, in any case, write a computer program to simulate the random walk and then fit your simulation results. Plot $P(\zeta)$ and $P'(\zeta)$, and comment on the results. What is $P'(1/2)$, the probability (density) that the walker spends roughly half his time on one side and half on the other?

4. Consider a "geometric Pearson walk" in two dimensions, in which the walker starts at the origin and takes steps of decreasing length a^n and (uniform) random angles, where $0 < a < 1$. Note that the walker must converge to a single final resting point (unlike the usual Pearson walk $a = 1$) at a random distance r_∞ from the origin. Write a computer program to determine the probability density $p(r_\infty)$, i.e. Prob.$(r < r_\infty < r + \Delta r) = 2\pi r p(r) \Delta r$. What is the shape of $p(r)$?

   For more fun, you can also study this problem in one dimension. It turns out that analytical results are possible. The dependence on r is particularly interesting.