A1. Nernst-Planck Behavior

Write a random walker simulation (you can use one of the previous solutions as a starting point) that includes the effects of electric force assuming that the particles in the simulation are charged and that an electric field is present. In other words, model the situation of electrophoretic flux. Probably the easiest way to do this is to periodically (not every time step though), move all of the walkers one bin to the left (or right, pick a direction for your force). You’ll want to restrict the walkers to a finite domain.

- If you start with a sharp distribution initially, how does it evolve?
  Answer: The peak drifts in the direction of the force as it is spreading out.

- What is the equilibrium configuration? (You may want to start your simulation with a “soft” distribution to hasten the evolution towards equilibrium.)

  Answer: The final configuration looks something like a decaying exponential, bunched up on the left side in the direction the electric force was pushing the walkers.
In[19]:=

(* Number of walkers *)
Nwalkers = 5000;

(* Number of time steps *)
Nts = 200;
driftfreq = 10;

(* The array will store the position of each walker *)
walkers = Table[0, {i, 1, Nwalkers}];

(* Array to store entropy at each time step *)
entropy = Table[0, {i, 1, Nts}];

(* Start the walkers in a tight (but not too tight) Gaussian to begin with *)
walkers = Round[RandomVariate[NormalDistribution[0, 1], Nwalkers]];

(* Makes a plot that is dynamically updated as the positions change *)
Dynamic[Histogram[walkers, {-20, 20, 1}, PlotRange -> {0, Nwalkers/10}]]

(* Guts of the program. Loop over all the time steps. For each time, loop over each walker position *)
For[j = 1, j < Nts, j++,

(* Calculate the entropy *)
For[i = 1, i <= Nwalkers, i++,
    walkers[i] = walkers[i] + RandomChoice[{-1, 1}];
    If[Mod[j, driftfreq] == 0, walkers[i] = 1];

(* keep the walkers "in the box" *)
walkers[i] = Min[walkers[i], 20];
walkers[i] = Max[walkers[i], -20];
]
]
Do problem 4.4 in the text

From the plot of $D$ as a function of $1/R$, we find that $D$ is inversely proportional to $a$ (see the plot below). This makes sense if we combine the Einstein relation, $\zeta D = k_B T$ and the coefficient of viscous friction, $\zeta = 6\pi \eta r$ (for a spherical particle) we get: $D = k_B T/(6\pi \eta r)$. At room temperature, this would give a $D$ of 0.22. From our fit to the data, we get 0.18. Not bad.