Physics 212 — Problem Set 2

Solutions

1.) a.) There are many way to generate random walk numerically, given a "random number generator", an algorithm that gives minimally correlated numbers between 0 and 1. Let such an algorithm be ran(). Then

$$x_{i+1} = x_i + (\mathrm{ran}() - \tfrac{1}{2})$$
$$y_{i+1} = y_i + (\mathrm{ran}() - \tfrac{1}{2})$$

gives the walker requested in the problem.

The implementation for the java GUI posted on the course Web site is given on the next page.

On the following page, you will see screen shots of the endpoints of 100 random walks with 10, 1000, 100000 steps. The scale in each picture is changed by a factor 10.

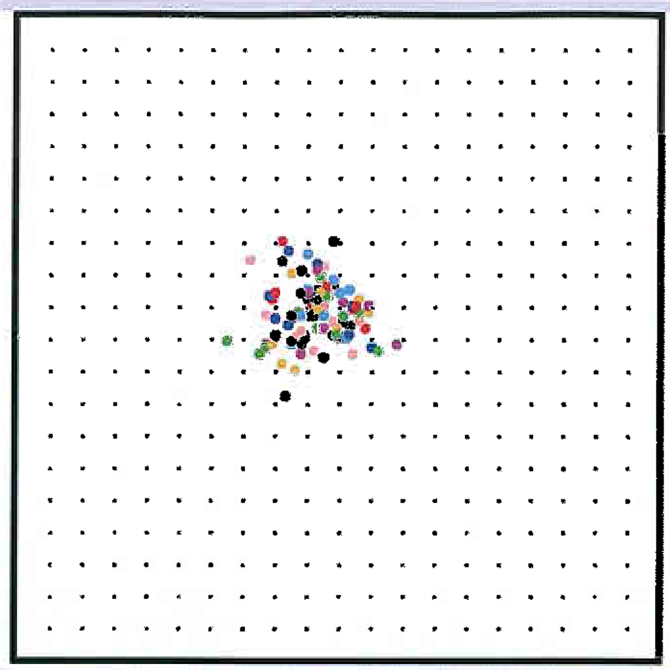
b.) On the page after that, you will see screen shots of 10,000 random walks with N=1 and N=10. The emergent rotational symmetry sets in quickly!

```
import java.awt.*;
import java.awt.event.*;
import java.applet.Applet;

public class myrandomwalk extends myrandomwalkGUI {


    int Ns;

    void solve(){
        /* basic conditions */
      Nw = 1000;
      Ns = 1000;
         /*  begin:   */
      Nsteps = 0;
      while(Nsteps < Ns){
         Nsteps++;
         for (int i = 0; i < Nw; i++){
            step(i);
         }
         refreshPicture();
         if (timetostop) break;
      }
      HPlot.refresh();
    }


    /* step uses the following equipment:

           ran() returns a random number (double) between 0 and 1
           Each time ran() is called, it returns a new random number.

           the position of the walker i is:

                      (xposition[i], yposition[i])

                                                                    */

    void step(int i){
        xposition[i] += ran() - 0.5;
        yposition[i] += ran() - 0.5;
     }

    double plotfunction(double x){
        /* this function is plotted in the right-hand display */
      double sigma = Math.sqrt(Ns/12.0);
      return  Nw / Math.sqrt(2.0* Math.PI * sigma * sigma)
                     * Math.exp(- x*x/(2.0 * sigma * sigma));
    }

}
```

100 walkers

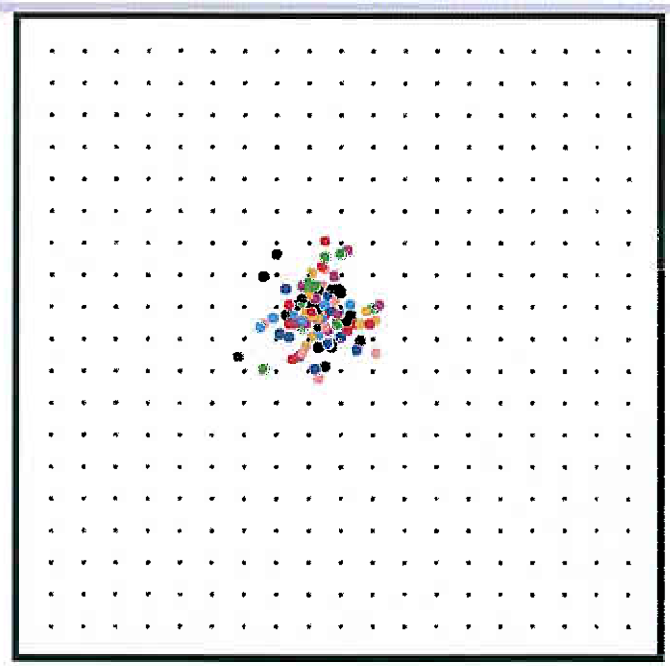
10 steps

10 X 10 box



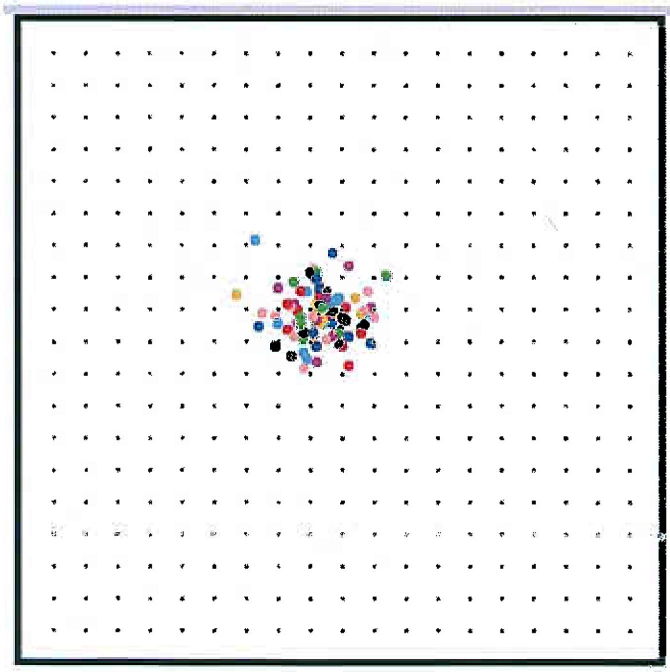
1000 steps

100 x 100 box

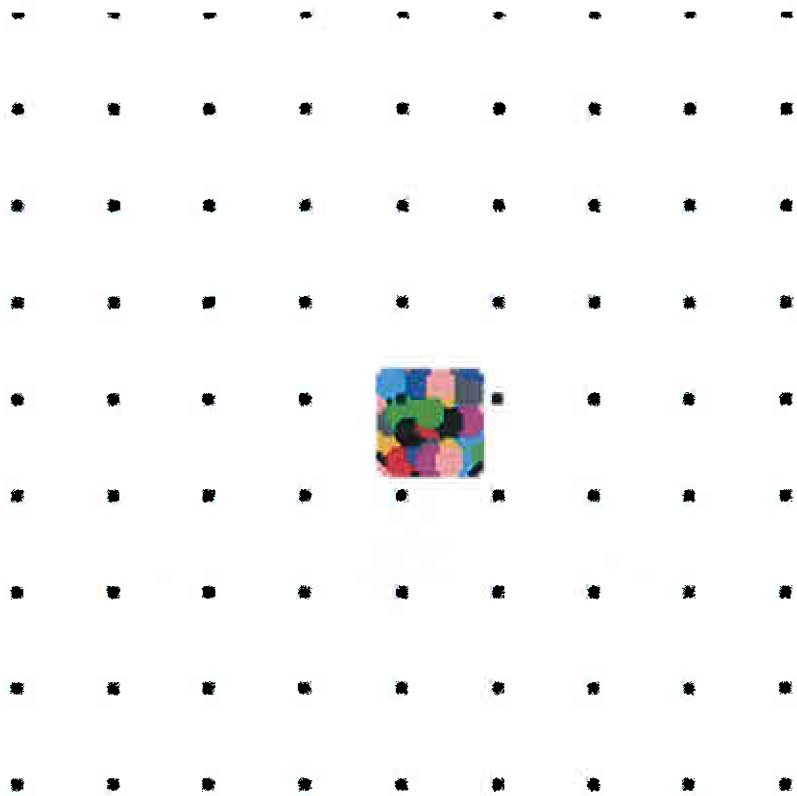


100000 steps

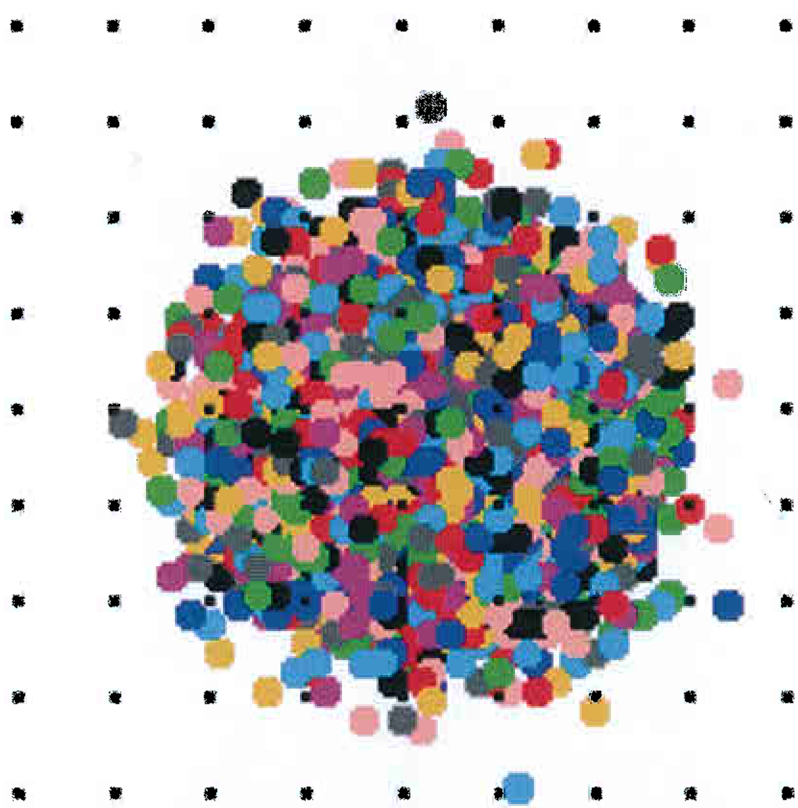
1000 x 1000 box



1 step



10 steps



c.) For 1-d steps uniformly distributed in $(-\frac{1}{2}, \frac{1}{2})$ the RMS step size is

$$\langle x^2 \rangle = \int_{-1/2}^{1/2} dx\, x^2 = 2 \cdot \frac{1}{3} \cdot \frac{1}{4} = \frac{1}{12}$$

or $RMS = \frac{1}{\sqrt{12}}$. Then $\sigma = \sqrt{N}/\sqrt{12}$

on the next page, there are screen shots of the function

$$\rho(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-x^2/2\sigma^2\right]$$

plotted against histograms of 10,000 random walks, for $N = 1, 2, 3, 5$.

2.) a.) $\left\langle \frac{p_z^2}{2m} \right\rangle = \frac{1}{2} k_B T$

so $\sqrt{\langle v_z^2 \rangle} = \left(\frac{k_B T}{m}\right)^{1/2}$

For an isothermal atmosphere at $T = 300°K$, $k_B T = 4.1 \times 10^{-14}$ erg

$m_{O_2} = 5.3 \times 10^{-23}$ g $\qquad m_{H_2} = 3.3 \times 10^{-24}$ g

so

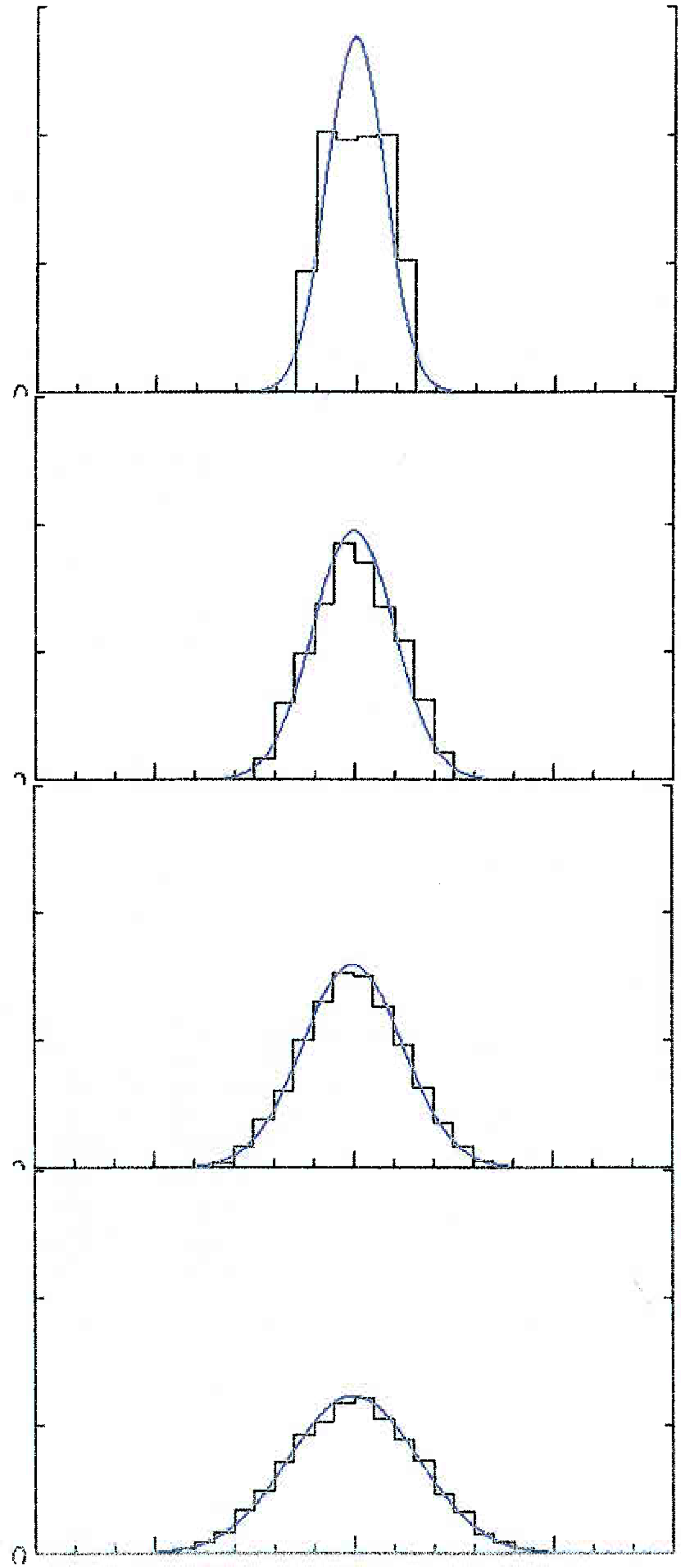
	O_2:	H_2
$\bar{v} = \sqrt{\langle v_z^2 \rangle}$	2.8×10^4 cm/sec	1.1×10^5 cm/sec
$h = \frac{1}{2}\frac{\bar{v}^2}{g}$	4.0×10^5 cm $= 4$ km	6.4×10^6 cm $= 64$ km
$t = 2\left(\frac{2h}{g}\right)^{1/2}$	57 sec	230 sec

1 step

2 steps

3 steps

5 steps



b) For $P(v) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-v^2/2\sigma^2}$

the probability of $v > v_e \gg \sigma$ is

$$P(v>v_e) = \int_{v_e}^{\infty} dv \frac{1}{\sqrt{2\pi\sigma^2}} e^{-v^2/2\sigma^2}$$

$$= \int_{v_e/\sqrt{2}\sigma}^{\infty} dt \frac{1}{\sqrt{\pi}} e^{-t^2}$$

$$= \frac{1}{\sqrt{2\pi}} \frac{\sigma}{v_e} e^{-v_e^2/2\sigma^2}$$

[Proof: $\int_x^{\infty} dt \frac{1}{\sqrt{\pi}} e^{-t^2} = \int_x^{\infty} \frac{dt}{\sqrt{\pi}} \frac{1}{2t}(2t e^{-t^2})$ integrate by parts

$$= -\frac{1}{2t\sqrt{\pi}} e^{-t^2}\Big|_x^{\infty} + \int \frac{dt}{\sqrt{\pi}}\left(-\frac{1}{2t^2}\right) e^{-t^2}$$

$$= \frac{1}{2\sqrt{\pi}\,x} e^{-x^2} + \mathcal{O}\left(\frac{e^{-x^2}}{x^3}\right) \quad]$$

then $\log P(v>v_e) = -\frac{v_e^2}{2\sigma^2} - \log\frac{v_e}{\sigma} - \frac{1}{2}\log 2\pi$

then for $v_e = 11$ km/sec

	O_2	H_2
v_e/σ :	39.	10.
$\log(P(v>v_e))$	$-765.$	$-53.$
$P(v>v_e)$	10^{-332}	10^{-23}

c.) Under Sethna's assumptions that the molecules thermalize only when they hit the ground:

	O_2	H_2
thermalizations / yr	5×10^5	1×10^5
fraction lost / yr	10^{-326}	10^{-18}
fraction lost / 4.5 Byr	10^{-316}	10^{-8}

For a more realistic thermalization time of $\sim10^{-5}$ sec from molecule-molecule collisions

thermalization / yr	3×10^{12}	3×10^{12}
fraction lost / yr	10^{-320}	10^{-11}
fraction lost / 4.5 Byr	10^{-310}	$\underline{10^{-1}}$

i.e. $O(1)$!

3.) a.) Area allowed for first disk: A

for 2^{nd} disk: $A-\pi(2r)^2$

for 3^{rd} disk: $A-2\cdot\pi(2r)^2$

so all

$$\Omega_V = \frac{1}{N!}\int dx\ \Theta(|\vec{x}_i-\vec{x}_j|>2r) = \frac{1}{N!}A(A-4\pi r^2)(A-8\pi r^2)$$

$$\cdots(A-(N-1)4\pi r^2)\cdots$$

b.) $S_Q = \log Q_V = \log \frac{A^N}{N!} + \sum_{m=0}^{N-1} \lg\left(1 - m\frac{4\pi r^2}{A}\right)$

so long as $N \cdot 4\pi r^2 \ll A$ (dilute approx.)

we can just expand the log

$$\sum_{m=0}^{N-1} \lg\left(1 - m\frac{4\pi r^2}{A}\right)$$

$$= \sum_{m=0}^{N-1}\left(-m\frac{4\pi r^2}{A} - \frac{1}{2}m^2\left(\frac{4\pi r^2}{A}\right)^2 + \cdots\right)$$

$$\approx \frac{N(N-1)}{2}\frac{4\pi r^2}{A}\left(1 + O\left(N\frac{4\pi r^2}{A}\right)\right)$$

$$\approx N\log\left(1 - N\cdot\frac{2\pi r^2}{A}\right)$$

then

$$S_Q = N\lg A - N\lg N + N + N\lg\left(1 - N\frac{2\pi r^2}{A}\right)$$

$$= N\lg(A - 2\pi r^2 N)$$

c.) $\frac{P}{T} = \left.\frac{\partial S}{\partial A}\right|_{E,N} = N\cdot\frac{1}{A - 2\pi r^2 N}$

or $P = \frac{NT}{A - bN}$ $\quad b = 2\pi r^2$

this goes to the ideal gas law as $b \to 0$ but is <u>stiffer</u> for nonzero b.

4.) Consider a system of two coupled microcanonical systems.

$$\Omega = \int dE \; e^{S_1(\mathcal{E}-E)} e^{S_2(E)}$$

$\mathcal{E}$ = total energy. The integral is steeply maximized at

$E = E_2 = E_*$ $\qquad$ $\mathcal{E} - E_* = E_1$

let $\quad \Delta E = E - E_*$

$$\Omega = e^{S(E_1)} e^{S_2(E_2)} \int d(\Delta E) \exp\left[\frac{\partial S_1}{\partial E}(-\Delta E) + \frac{1}{2}\frac{\partial^2 S_1}{\partial E^2}(-\Delta E)^2 + \cdots + \frac{\partial S_2}{\partial E}(\Delta E) + \frac{1}{2}\frac{\partial^2 S_2}{\partial E^2}(\Delta E)^2 + \cdots \right]$$

$\frac{\partial S_1}{\partial E} = \frac{\partial S_2}{\partial E}$ for equilibrium, so

$$= e^{S_1(E_1) + S_2(E_2)} \int d(\Delta E) \exp\left[\frac{1}{2} \underbrace{\left(\frac{\partial^2 S_1}{\partial E^2} + \frac{\partial^2 S_2}{\partial E^2} \right)} \Delta E^2 \right]$$

E_* represents a max so this is negative

$$\sigma_E^2 = -\left(\frac{\partial^2 S_1}{\partial E^2} + \frac{\partial^2 S_2}{\partial E^2} \right)^{-1}$$

a.) $\left(\frac{\partial S}{\partial E}\right)_{V,N} = \frac{1}{T}$ so $\left(\frac{\partial^2 S}{\partial E^2}\right)_{V,N} = \left(\frac{\partial T}{\partial E}\right)_{V,N}\left(-\frac{1}{T^2}\right)$

$$= -\frac{1}{N c_v T^2}$$

b.) then

$$\sigma_E^2 = -\left(\frac{-1}{N_1 c_v^{(1)} T^2} + \frac{-1}{N_2 c_v^{(2)} T^2}\right)^{-1}$$

if $N_1 = N_2 = N$

$$\sigma_E^2 = N T^2 \left(\frac{1}{c_v^{(1)}} + \frac{1}{c_v^{(2)}}\right)^{-1}$$

c.) In a classical simulation, there will be a configurational entropy that affects the thermodynamics, but the kinetic energy will obey

$$K = \langle \text{kin.} E \rangle = \frac{3}{2} N T$$

exactly!

The total specific heat will be

$$c_v = c_v^{(kin)} + c_v^{(config)} \qquad c_v^{kin} = \frac{1}{N}\frac{\partial K}{\partial T} = \frac{3}{2}$$

$$\sigma_E^2 = N T^2 \left(\frac{1}{c_v^{(kin)}} + \frac{1}{c_v^{conf.}}\right)^{-1}$$

$$= N T^2 \left(\frac{2}{3} + \frac{1}{c_v^{config}}\right)^{-1}$$

$$= \left(\frac{2K}{3}\right)^2 \frac{1}{N} \left(\frac{2}{3} + \frac{1}{c_v^{config}}\right)^{-1}$$

then $$\frac{2}{3} + \frac{1}{c_v^{(config)}} = \left(\frac{2K}{3}\right)^2 \frac{1}{N} \frac{1}{\sigma_E^2}$$

$$c_v^{(\text{contig})} = \left[\frac{4}{9} \frac{K^2}{N\sigma_\varepsilon^2} - \frac{2}{3} \right]^{-1}$$

then

$$c_v = \frac{3}{2} + \left[\frac{4}{9} \frac{K^2}{N\sigma_\varepsilon^2} - \frac{2}{3} \right]^{-1}$$

5.) a.) For 1 particle:

Prob in $V = \frac{1}{K}$ Prob not in V $\frac{K-1}{K}$

For 2 particles

Prob of 2 in V: $\frac{1}{K^2}$ 1 in V 1 not: $2 \cdot \frac{1}{K} \frac{K-1}{K}$

both not: $\left(\frac{K-1}{K}\right)^2$ sum $= 1$

For T particles.

Prob of n particles in V $T-n$ not:

$$\mathbb{P}(n) = \frac{T!}{n!(T-n)!} \left(\frac{1}{K}\right)^n \left(\frac{K-1}{K}\right)^{T-n}$$

check

$$\sum_{n=0}^{T} \mathbb{P}(n) = \sum_{n=0}^{T} \binom{T}{n} \left(\frac{1}{K}\right)^n \left(\frac{K-1}{K}\right)^{T-n} = \left(\frac{1}{K} + \frac{K-1}{K}\right)^T = 1$$

✓

b.) $$\rho_n = \frac{a^n e^{-a}}{n!}$$

$$\sum_{n=0}^{\infty} \rho_n = e^{-a} \sum_{n=0}^{\infty} \frac{a^n}{n!} = e^{-a} e^{a} = 1 \quad \checkmark$$

$$\langle n \rangle = \sum_{n=0}^{\infty} n\rho_n = e^{-a} \sum_{n=0}^{\infty} \frac{n a^n}{n!} = e^{-a} \sum_{n=1}^{\infty} \frac{a^n}{(n-1)!}$$

$$= e^{-a} a e^{a} = a$$

$$\langle n(n-1) \rangle = \sum_{n=0}^{\infty} n(n-1)\rho_n = e^{-a} \sum_{n=0}^{\infty} \frac{n(n-1)\, a^n}{n!} = e^{-a} \sum_{2} \frac{a^n}{(n-2)!}$$

$$= e^{-a} a^2 e^{a}$$

so

$$\langle n \rangle = a \qquad \langle n^2 - n \rangle = a^2 \Rightarrow \langle n^2 \rangle = a^2 + a$$

$$\langle n^2 \rangle - \langle n \rangle^2 = a$$

c.) Now let $K, T \to \infty$ in the formulae of part (a)

$$\frac{T!}{(T-n)!} \approx T^n \qquad \left(\frac{K-1}{K}\right)^{T-n} = \left(1 - \frac{1}{K}\right)^T \approx e^{-T/K}$$

if $T/K \to$ const as $T, K \to \infty$. T is the total number of particles, so T/K is the expected # of particles in the subvolume of fraction K. Write

$$T/K \to N_0 \quad \text{as} \quad T, K \to \infty$$

then $$\mathbb{P}(n) \to \frac{1}{n!}\left(\frac{T}{K}\right)^n e^{-T/K} = \frac{1}{n!}(N_0)^n e^{-N_0}$$

so

$$\mathcal{P}(n) \to \rho_n \quad (a = N_0)$$

d.) Now set $n = N_0 + m$ assume $N_0 \gg m$

$$\mathcal{P}(N_0+m) = \frac{T!}{(N_0+m)!(T-N_0-m)!} \left(\frac{1}{K}\right)^{N_0+m} \left(\frac{K-1}{K}\right)^{T-N_0-m}$$

For simplicity, use $n! = n^n e^{-n}$ or $\log n! = n\log n - n$

we can fix this later.

$$\log \frac{T!}{(N_0+m)!(T-N_0-m)!} = T\log T - \cancel{T} - (N_0+m)\log(N_0+m) + \cancel{(N_0+m)}$$
$$- (T-N_0-m)\log(T-N_0-m) + \cancel{(T-N_0-m)}$$

$$= T\log T - (N_0+m)\log N_0 - (N_0+m)\left[\frac{m}{N_0} - \frac{1}{2}\frac{m^2}{N_0^2} + \dots\right]$$
$$- (T-N_0-m)\log(T-N_0) - (T-N_0-m)\left[\frac{-m}{T-N_0} - \frac{1}{2}\frac{m^2}{(T-N_0)^2} + \dots\right]$$

$$= T\log T - N_0\log N_0 - (T-N_0)\log(T-N_0)$$
$$- m\log\left(\frac{N_0}{T-N_0}\right)$$
$$- m - \frac{m^2}{N_0} + \frac{1}{2}\frac{m^2}{N_0} + m - \frac{m^2}{(T-N_0)} + \frac{1}{2}\frac{m^2}{(T-N_0)} + \dots$$

$$= T\log T - N_0\log N_0 - (T-N_0)\log(T-N_0)$$
$$- m\log\left(\frac{N_0}{T-N_0}\right) - \frac{1}{2}m^2\left(\frac{1}{N_0} + \frac{1}{T-N_0}\right) + \dots$$

then

$$\log P(N_0+m) = T\log T - N_0\log N_0 - (T-N_0)\log(T-N_0)$$
$$- m\log\left(\frac{N_0}{T-N_0}\right) - \frac{1}{2}m^2\,\frac{T}{N_0(T-N_0)}$$
$$-(N_0+m)\log K - (T-N_0-m)\log\frac{K}{K-1}$$

set $K = T/N_0$; then the third line becomes

$$-N_0\log\left(\frac{T}{N_0}\right) - (T-N_0)\log\left(\frac{T}{T-N_0}\right) - m\log\left(\frac{T}{N_0}\,\frac{T-N_0}{T}\right)$$

all that remains after the cancellation is

$$\log P(N_0+m) = -\frac{1}{2}\,\frac{T}{N_0(T-N_0)}\,m^2$$

so
$$\sigma_K^2 = \frac{N_0(T-N_0)}{T} = N_0\left(1-\frac{1}{K}\right)$$

$$\sigma_2^2 = \frac{N_0}{2} \qquad \sigma_\infty^2 = N_0$$

e.) Finally, clean up the normalization. This requires using a better approximation for the factorial

$$\log n! = n\lg n - n + \tfrac{1}{2}\lg n + \tfrac{1}{2}\lg 2\pi$$
$$= (\text{previous}) + \tfrac{1}{2}\log(2\pi n)$$

then

$$\log \mathcal{P}(N_0+m) = (\text{previous}) + \tfrac{1}{2}\log 2\pi T - \tfrac{1}{2}\log 2\pi(N_0+m)$$
$$\qquad - \tfrac{1}{2}\log 2\pi(T-N_0-m)$$

$$= (\text{previous}) - \tfrac{1}{2}\log 2\pi - \tfrac{1}{2}\log \frac{N_0(T-N_0)}{T}$$

then

$$\mathcal{P}(N_0+m) \cong \frac{1}{\sqrt{2\pi\sigma_k^2}}\, e^{-m^2/2\sigma_k^2}$$

where $$\sigma_k^2 = \frac{N_0(T-N_0)}{T}$$

This is properly normalized.