P114 Seminar #6 - Problem 1
Alternate Prob 1
G+T Problem 4.38

Solutions for Week 6

$N_A = 4 \quad E_A = -2\mu B$
$N_B = 16 \quad E_B = -2\mu B$

a) $\Omega = \Omega_A \Omega_B \qquad \Omega = \frac{N!}{n!(N-n)!} \qquad n = \frac{N}{2} - \frac{E}{2\mu B} \qquad n_a = 4/2 - \frac{-2\mu B}{2\mu B} = 3$

$n_b = 16/2 - \frac{-2\mu B}{2\mu B} = 9$

$\Omega_A = \frac{4!}{3!(4-3)!} = \frac{24}{6 \cdot 1} = 4$

$\Omega_B = \frac{16!}{9!(16-9)!} = 11440$

$\Omega = 4 \times 11440 = \boxed{45760}$

b) $\Omega(E) = \sum_{E_A} \Omega_A(E_A)\Omega_B(E-E_A) \qquad E = E_A + E_B = -4\mu B$

and n_A and n_B must be integers

$P_A(E_A) = \frac{\Omega_A(E_A)\Omega_B(E-E_A)}{\Omega(E)}$

$E_A = 0\mu B \; n_A = 2, \; n_B = 10, \; E_B = -4\mu B$
$E_A = -4\mu B \; n_A = 4, \; n_B = 8, \; E_B = 0\mu B$

$n_A = 0, \; n_B = 12$ can't go further

$n_A = 3, \; n_B = 9$
$\cancel{n_A = 3, \; n_B = 7}$ can't have -1!!
$n_A = 1, \; n_B = 11$

$\Omega(E) = \left(\frac{4!}{2!(2!)}\right)\left(\frac{16!}{10!(6!)}\right) + \left(\cancel{\frac{4!}{4!(0!)}}\right)\left(\frac{16!}{8!(8!)}\right) + \left(\frac{4!}{3!(1!)}\right)\left(\frac{16!}{9!(7!)}\right) + \left(\frac{4!}{1!(3!)}\right)\left(\frac{16!}{11!(5!)}\right) + \left(\cancel{\frac{4!}{0!(4!)}}\right)\left(\frac{16!}{12!(4!)}\right)$

$\Omega(E) = 48048 + 12870 + 45760 + 17472 + 1820$

$= 125970$

$P_A(E_A) = \frac{45760}{125970} \rightarrow E_A = -2\mu B \qquad \boxed{P_A(-2\mu B) = \frac{352}{969} \text{ or } 36.3\%}$

c) $\overline{E_A} = \cancel{\frac{48048}{125970}(0\mu B)} + \frac{12870}{125970}(-4\mu B) + \frac{45760}{125970}(-2\mu B) + \frac{17472}{125970}(2\mu B) + \frac{1820}{125970}(4\mu B)$

$\overline{E_B} = \frac{48048}{125970}(-4\mu B) + \cancel{\frac{12870}{125970}(0\mu B)} + \frac{45760}{125970}(-2\mu B) + \frac{17472}{125970}(-6\mu B) + \frac{1820}{125970}(-8\mu B)$

$\boxed{\overline{E_A} = -0.80\,\mu B \qquad \overline{E_B} = -3.2\,\mu B}$

$$\Delta E = \sqrt{\overline{E^2} - \overline{E}^2}$$

$\Rightarrow \quad \delta E_A = 1.80 \mu B$

$\Delta E_B = 1.80 \mu B$

Most probable macrostate is

E_A	E_B
-4	0
-2	-2
0	-4
2	-6
4	-8

Most probable

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Problem Solutions

1. Einstein solid + Magnetic System

G+T Problem 4.39

Einstein solid $N_A = 8$

$\Delta E = \pm 1$

Spin system $N_B = 8$

$\Delta E = \pm 1 \Rightarrow \mu B = 1/2$

Initially $E_A = 4$ $E_B = -1$

Find: Initial S? Then remove constraint + let systems exchange energy. Want to find $P_A(E_A)$, $\bar{E}_A$, σ_A^2, $\bar{E}_B$, σ_B^2, and prob that energy goes $A \to B$ and " " " " $B \to A$.

Which is initially hotter?

What is change in entropy (when equilib is reached?

Soln:

$$\Omega_A(E_A) = \frac{(E_A + N_A - 1)!}{E_A!\,(N_A - 1)!}$$

$$\Omega_B(E_B) = \frac{N_B!}{n!\,(N_B - n)!}$$

For given initial state, since $E_A = 4$

initially $\Omega_A = \frac{11!}{4!\,7!} \Rightarrow \ln \Omega_A = \ln(330) = 5.80$

while in general $\Omega_A(E_A) = \frac{(E_A+7)!}{E_A!\,7!}$

initially Since $(2n - N_B)\,(\mu B) = E_B$ $\frac{1}{2}$

$$-2n + N_B = 2E_B$$

$$N_B - 2E_B = 2n$$

initially

$$8 + 2 = 2n \;;\; n = 5$$

and in general

$$n = \frac{N_B}{2} - E_B$$

$$= 4 - E_B$$

so initially $\Omega_B = \frac{8!}{5!\,3!} = \ln(56) = 4.03$

and in general $\Omega_B(E_B) = \frac{8!}{(4-E_B)!\,(4+E_B)!}$

So initially $S = S_A + S_B = \underline{9.83\,k}$

After constraint is lifted, since $E = 4-1 = 3$

$$\Omega(E_A) = \Omega_A(E_A)\Omega_B(3-E_A) \quad \text{so}$$

$$P_A(E_A) = \frac{\Omega(E_A)}{\sum_{E_A=0}^{7} \Omega(E_A)}$$

where $\Omega = \Omega_A(E_A)\Omega_B(E-E_A)$

Note The highest E_A can be is 7 b/c the lowest E_B can be is -4, when all spins are up ... Thence $7-4=3$.

Lowest E_A can be is, of course, 0

E_A	Ω_A	E_B *	Ω_B	Ω +	$P_A(E_A)$
0	1	3	8	8	0.000117
1	8	2	28	224	0.00327
2	36	1	56	2016	0.0294
3	120	0	70	8400	0.123
4	330	-1	56	18480	0.270
5	792	-2	28	22176	0.324
6	1716	-3	8	13728	0.201
7	3432	-4	1	3432	0.050

* $E_B = 3 \Rightarrow n=1$
$E_B = 2 \Rightarrow n = 2$
etc...

+ $\Omega = \Omega_A \Omega_B$

Used Mathematica to get $\Omega_{tot} = 68{,}464$

Thenbook $P_A(E_A) \dfrac{\Omega_A(E_A)\Omega_B(3-E_A)}{\Omega}$

We can thus get values:

$$\bar{E}_A = \sum_{E_A=0}^{7} E_A P_A(E_A) = \underline{4.68}$$

$$\bar{E}_B = 3 - \bar{E}_A = -\underline{1.68}$$

Fluctuations:

$$\sigma_A^2 = \overline{E_A^2} - \overline{E}_A^2 = \sum E_A^2 P_A(E_A) - \overline{E}_A^2$$

$$= 23.3 - 4.68^2 = \underline{1.40}$$

$$\Rightarrow \sigma_A = \approx 1.18$$

Similarly

$$\overline{E_B^2} = \sum_{E_A=0}^{7} \qquad (3-E_A)^2 P_A(E_A)$$

Mathematica

$$= 4.215$$

$$\therefore \sigma_B^2 = \overline{E_B^2} - \overline{E}_B^2 = 1.39$$

$$\Rightarrow \underline{\sigma_B = 1.18}$$

Most probable energies:

$P_A(E_A)$ is max

$$\Rightarrow E_A = 5, \; E_B = -2$$

This state has entropy

$$S = S_A(E_A = 5) + S_B(E_B = -2)$$

$$= k \ln 22176 = 10.0k$$

So $\Delta S = k \ln 22176 - k \ln 8 = \underline{k \cdot 7.927}$

Prob E goes $A \to B$ is

$$P_A(3) + P_A(2) + P_A(1) = \underline{0.156}$$

higher prob so B

Prob E goes $B \to A$ is

$$P_A(5) + P_A(6) + P_A(7) = \underline{0.270}$$

States! Hotter A colder!

2) Harmonic Oscillators in canonical ensemble ...

$$Z = \frac{e^{-\beta\hbar\omega/2}}{1-e^{-\beta\hbar\omega}}$$

$f, s, \bar{e}$ wanted

$$S = -\left(\frac{\partial f}{\partial T}\right)_V = -k\left[\ln\left(1-e^{-\beta\hbar\omega}\right) - \right.$$

$$\left. -\left(\frac{\hbar\omega}{\beta}\right)e^{-\beta\hbar\omega}/\left(1-e^{-\beta\hbar\omega}\right)\right]$$

$$f = -kT\ln Z$$

$$= -\tfrac{1}{2}\hbar\omega + kT\ln\left(1-e^{-\beta\hbar\omega}\right)$$

$$\bar{e} = -\frac{d}{d\beta}\ln Z = \left(\frac{1}{2}\hbar\omega + \frac{\hbar\omega}{\left(e^{\beta\hbar\omega}-1\right)}\right)N$$

3) G + T 4.50 1D SHO with

heat bath...

(a) Find C : Since $\ln Z = -\left(\frac{\beta\hbar\omega}{2} - \ln(1-e^{-\beta\hbar\omega})\right)$

(from an earlier problem)

per particle $\bar{E} = \hbar\omega\left[\frac{1}{2} + \frac{1}{e^{\beta\hbar\omega}-1}\right]$ (also earlier problem)

Thus $C = \frac{\partial \bar{E}}{\partial T} = \frac{\partial \bar{E}}{\partial \beta}\frac{\partial \beta}{\partial T} = -\frac{1}{kT^2}\frac{\partial \bar{E}}{\partial \beta} = k\left(\frac{\hbar\omega}{kT}\right)^2 \frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}$

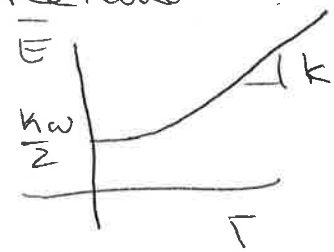
C per particle

(b) Plot the T dependence of

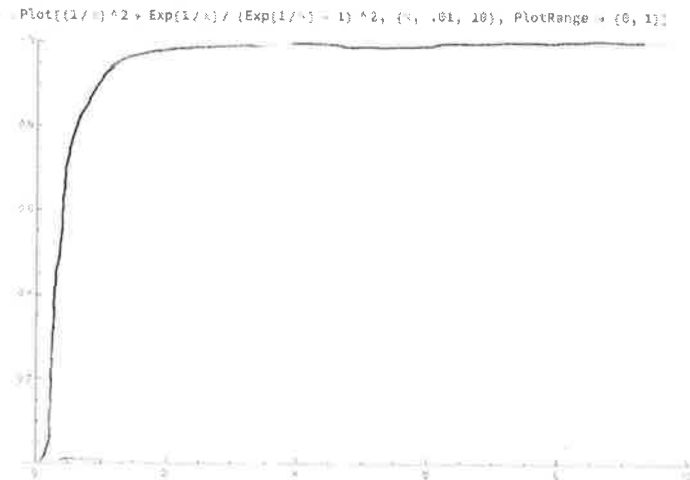
E & C ... show that as $T \to \infty$

$E \to kT$ and $C \to k$

Sorry, I have no plot of E(T) but freehand it:



Here is C:



X

$x = kT$

c) To Show: As $T \to 0$ ie $\hbar\omega \gg kT$

$\bar{E} \cong \hbar\omega(\frac{1}{2} + e^{-\beta\hbar\omega})$. Find C

Why so much smaller than at high T?

Why so different from 2-state system?

Answer: $\beta\hbar\omega \gg 1$ is this low-T limit.

There $e^{\beta\hbar\omega} - 1 \simeq e^{\beta\hbar\omega}$

$\Rightarrow \bar{E} \simeq \hbar\omega\left[\frac{1}{2} + e^{-\beta\hbar\omega}\right]$ ✓

Also $C = -\frac{1}{kT^2}\frac{\partial \bar{E}}{\partial \beta} = \frac{\hbar\omega}{kT^2}(\hbar\omega)e^{-\beta\hbar\omega}$

$$= k\left(\frac{\hbar\omega}{kT}\right)^2 e^{-\beta\hbar\omega}$$

So $C \to 0$ exponentially!

INTERLUDE

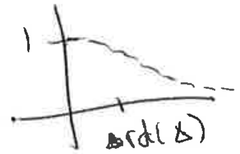
For 2 state system wisdom, we could solve G+T 4.47 or see example in B+B ch 20 where $E = 0$ or Δ. Here is calculn:

G+T 4.47 →

(a) T dep of $p(0)$ + $p(1)$ for 1 particle?

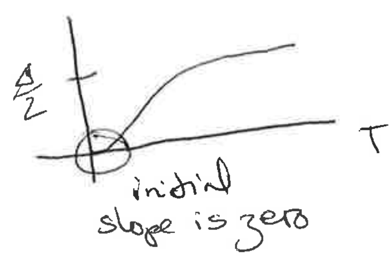
Here $Z_1 = (1+e^{-\beta\Delta})$; $Z_N = (1+e^{-\beta\Delta})^N$

so $P(0) = \frac{1}{1+e^{-\beta\Delta}}$; $P(1) = \frac{e^{-\beta\Delta}}{1+e^{-\beta\Delta}}$

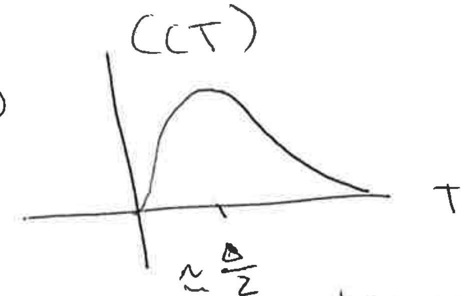


$P(0)+P(1) = 1$

(b) $\bar{E}(T)$



(c)



C is: zero at low + high T. At low T, first excited state is too high to access. At high T, there is nowhere else to go... energy is evenly distributed

(d) $Z_1 = (1+e^{-\beta\Delta})$; $f = -kT\ln Z_1 = -kT\ln(1+e^{-\Delta/kT})$

$\bar{e} = \frac{\partial \beta f}{\partial \beta} = \frac{\Delta}{e^{\beta\Delta}+1}$ Check: $T\to 0$ means $\beta\to\infty \Rightarrow \bar{e}\to 0$

$T\to\infty$ means $\beta\to 0 \Rightarrow \bar{e}\to\frac{\Delta}{2}$ ✓

$$C = \frac{\partial \bar{e}}{\partial T} = -\frac{1}{T^2}\frac{\partial}{\partial\beta}\frac{\Delta}{e^{\beta\Delta}+1} = \left(\frac{\Delta}{kT}\right)^2\frac{e^{\Delta/kT}}{(e^{\Delta/kT}+1)^2}$$

Check: $T \to 0$ means $\beta \to \infty \Rightarrow C \to 0$ B03

via the exponential in denom

$T \to \infty$ means $\beta \to 0 \Rightarrow C \to 0$

via the $\frac{1}{T^2}$

Back to G+T 4.50

(d) $T \to 0$, $S \to 0$

$$S_{SHO} = k\left[\frac{\beta\hbar\omega}{\underbrace{e^{\beta\hbar\omega}-1}_{\to 0}} - \underbrace{\ln(1-\underbrace{e^{-\beta\hbar\omega}}_{\to 0})}_{\ln 1 \to 0}\right]$$

$T \to \infty$ means $\beta \to 0$

so $$S_{SHO} = k\left[1 - \ln(\beta\hbar\omega)\right]$$

$$\simeq k\left[\underbrace{1}_{\text{unimpt}} + \ln\frac{kT}{\hbar\omega}\right]$$

$$\simeq k\ln\frac{kT}{\hbar\omega}$$

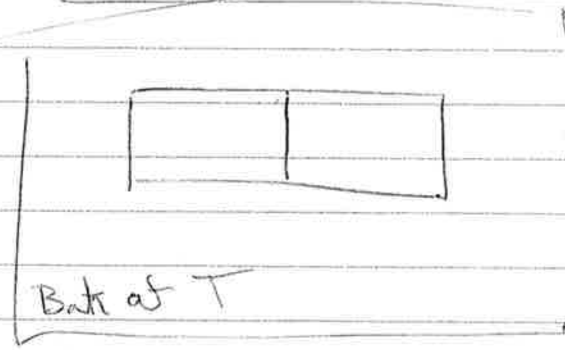
one particle

for N we have

$$Nk\ln\frac{kT}{\hbar\omega}$$

Problem 4

G+T Problem 4.52



Particles are Distinguishable
2 particles
2 boxes

Single particle i has energy $e_i = 0$ left box, $e_i = r$ right box

Further, if both particles are in same box, system has add'l energy Δ.

(a) Count up $4 = 2^2$ μstates

Particle 1	Part 2	Energy
l	l	Δ
l	r	r
r	l	r
r	r	$2r+\Delta$

(b) $$Z = e^{-\beta\Delta} + 2e^{-\beta r} + e^{-\beta(2r+\Delta)}$$

And mean energy is

$$E = \frac{\Delta e^{-\beta\Delta} + 2re^{-\beta r} + (2r+\Delta)e^{-\beta(2r+\Delta)}}{e^{-\beta\Delta} + 2e^{-\beta r} + e^{-\beta(2r+\Delta)}}$$

(c) Prob of any microstate?

$$P(\ell,\ell) = e^{-\beta\Delta}/Z$$

$$P(\ell,r) = e^{-\beta r}/Z$$

$$P(r,\ell) = e^{-\beta r}/Z$$

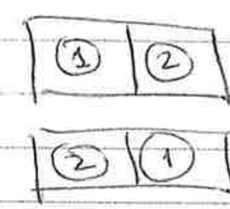
$$P(r,r) = e^{-\beta(2r+\Delta)}/Z$$

(d) Spose $r=1$ + $\Delta=15$.

Qualitative sketch of C ...

Limits: • Low T, particles adopt one of lowest energy ~~states with~~ $E = 2r$

And $C \to 0$



-or-

• High T, states are evenly occupied so again $C \to 0$ $\quad E = \frac{\Delta+2r+2r+\Delta}{4}$

• C will rise from zero and have a maximum when particles are starting to get enough energy to share same box. This is $E=15$ (left box) or $E=17$ (right box)

So each particle has around $\frac{E}{2} = 7\frac{1}{2}$ energy. So guess when $kT \approx 7$ or 8 ...

CV

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Plot[EE'[T], {T, .01, 30}]
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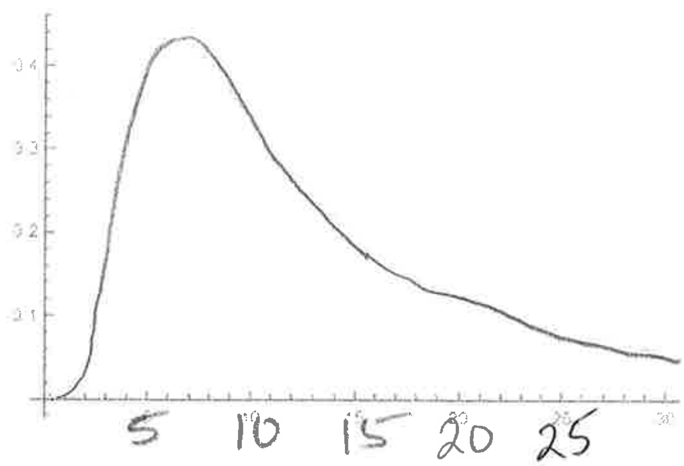


Problem 5

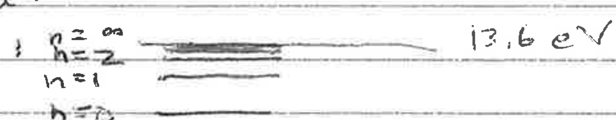
Hydrogen:

i) B+B 20.8

Energies are $E = -R/n^2$ $R = 13.8$ eV

and $g(E) = 2n^2$

(a)



(b) To show: $Z = \sum_{n=1}^{\infty} 2n^2 e^{R/n^2kT}$

This is just a matter of definition

since $$Z = \sum_{E_i} g(E_i) e^{-\beta E_i}$$

Let's now just assume first 2 states are populated ...

$$Z \approx \sum_{n=1}^{2} 2n^2 e^{-\beta R/n^2}$$

What is $\bar{E}$ at $T = 300K$?

$$\bar{E} = \sum E P(E) = \sum_{n=1}^{2} 2n^2 \left(\frac{-R}{n^2}\right) e^{-\beta R/n^2}$$

with $kT \approx \frac{1}{40}$ eV, $P(n=1) = \frac{2e^{-\beta R}}{2e^{-\beta R} + 8e^{-\beta R/4}}$

15

Thus, $P(n=1) = \frac{1}{1+4e^{\frac{3R}{4kT}}} = \frac{1}{1+4e^{3/4 \cdot 13.6 \cdot 40}}$

≈ 1

Clearly, $\bar{E} = E_1 = -R = -13.6\,eV$

Problem 6

B+B 21.4

Two state system with degeneracy

Atom in solid

$$\begin{array}{ll} & g_2 \;\text{———} \\ g_1 \;\text{———} & \end{array} \Big\} \Delta$$

<u>To show</u>: $Z_{atomic} = g_1 + g_2 e^{-\beta\Delta}$

and $$C_{atomic} = \frac{g_1 g_2 \Delta^2 e^{-\beta\Delta}}{kT^2 (g + g_2 e^{-\beta\Delta})^2}$$

Also, if monatomic gas of these atoms exists, since $Z_N = Z_1^N / N!$ and $Z_1 = Z_{atomic} Z_{trans}$ with $Z_{trans} = \frac{V}{\lambda_{th}^3}$, WTS that

$$C = N\left[\tfrac{3}{2}k + \frac{g_1 g_2 \Delta^2 e^{-\beta\Delta}}{kT^2 (g_1 + g_2 e^{-\beta\Delta})^2}\right].$$

Sol'n,

Clearly, $Z_{atomic} = \sum_s e^{-\beta E_s}$ μ states

$$= \sum_{E_j} g_j e^{-\beta E_j} \quad \text{energy state}$$

Thus it follows $Z_{atomic} = g_1 e^0 + g_2 e^{-\beta\Delta}$;

$Z_{atomic} = g_1 + g_2 e^{-\beta\Delta}$ QED

Now need specific heat ...

$$\bar{E} = U = -\frac{\partial \ln Z}{\partial \beta} = -\frac{1}{Z}\frac{\partial Z}{\partial \beta} = \frac{+g_2 \Delta e^{-\beta\Delta}}{g_1 + g_2 e^{-\beta\Delta}}$$

$$\therefore\ C = \frac{\partial U}{\partial T} \underset{\text{chain rule}}{=} \frac{\partial U}{\partial \beta}\frac{\partial \beta}{\partial T} = \frac{\partial U}{\partial \beta}\left(-\frac{1}{kT^2}\right)$$

Thus $$C = \frac{-(g_1 + g_2 e^{-\beta\Delta})\, g_2 \Delta^2 e^{-\beta\Delta} - g_2 \Delta e^{-\beta\Delta}\left(-g_2 \Delta e^{-\beta\Delta}\right)}{\left(g_1 + g_2 e^{-\beta\Delta}\right)^2} \times \left(\frac{-1}{kT^2}\right);$$

Thus
$$C = \left(\frac{1}{kT^2}\right)\frac{g_1 g_2 \Delta^2 e^{-\beta\Delta}}{\left(g_1 + g_2 e^{-\beta\Delta}\right)^2} = \frac{g_1 g_2 \Delta^2 e^{-\beta\Delta}}{kT^2\left(g_1 + g_2 e^{-\beta\Delta}\right)^2} \quad \text{QED}$$

Now for ideal gas, since

$$Z = Z_{\text{atomic}} Z_{\text{trans}}$$

$$U = -\frac{\partial}{\partial \beta}\ln Z = -\frac{\partial}{\partial \beta}\left[\ln Z_{\text{atomic}} + \ln Z_{\text{trans}}\right]$$

$$C = \frac{\partial U}{\partial T} = -\frac{\partial}{\partial T}\frac{\partial}{\partial \beta}\ln Z_{\text{atomic}} - \frac{\partial}{\partial T}\frac{\partial}{\partial \beta}\ln Z_{\text{trans}}$$

In other words, $C = C_{\text{atomic}} + C_{\text{trans}}$

So since we know

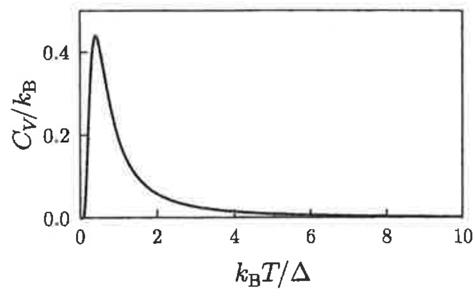
$$C_{trans} = \frac{3}{2}k^{*},$$

The result follows :)

Finally, comparison with Fig 20.4 part (a) ... This is a 2-state system w/o degeneracy:

B+B Eq. 20.25

$$C_V = k\left(\frac{\beta\Delta}{2}\right)^2 \operatorname{sech}^2\left(\frac{\beta\Delta}{2}\right)$$



vs.

ours

$$C = \left(\frac{1}{kT^2}\right)\frac{g_1 g_2 \Delta^2 e^{-\beta\Delta}}{(g_1+g_2 e^{-\beta\Delta})^2}$$

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* Reminder: $Z = \frac{V}{\lambda_{th}^3} = \frac{V(2\pi m k T)^{3/2}}{h^3} = \frac{V(2\pi m)^{3/2}}{h^3\beta^{3/2}}$

$$\therefore\ U = -\frac{1}{Z}\frac{\partial Z}{\partial \beta} = \frac{-1}{\left(\frac{V(2\pi m)^{3/2}}{h^3\beta^{3/2}}\right)}\left(-\frac{3}{2}\right)\frac{V(2\pi m)^{3/2}}{h^3\beta^{5/2}},$$

$$\therefore\ U = +\frac{3}{2}kT \Rightarrow C = \frac{3}{2}k$$:)

First of all, if $g_1 = g_2 = 1$ we'd have

$$C = \frac{k}{k^2T^2}\frac{\Delta^2}{e^{\beta\Delta}(1+e^{-\beta\Delta})^2} = k(\beta\Delta)^2\frac{1}{\left(e^{\frac{\beta\Delta}{2}}+e^{-\frac{\beta\Delta}{2}}\right)^2}$$

or $$C = k\left(\frac{\beta\Delta}{2}\right)^2\frac{1}{\operatorname{sech}^2\left(\frac{\beta\Delta}{2}\right)}$$ which agrees with B+B (20-25) :)

So let us rewrite B+B expression as

$$C = \left(\frac{1}{kT^2}\right)\frac{\Delta^2 e^{-\beta\Delta}}{(1+e^{-\beta\Delta})^2} \qquad \text{B+B (20.25)}$$

Our major differences are two:

- our numerator is larger by $g_1 \cdot g_2$.
- our denominator is weighted differently.

Let's let $g_2 = \alpha g_1$. Then we'd have

$$C = \left(\frac{1}{kT^2}\right)\frac{\alpha\Delta^2 e^{-\beta\Delta}}{(1+\alpha e^{-\beta\Delta})^2}$$

This makes sense. If α is small, gs is very much favored, and in fact $\alpha \to 0 \Rightarrow C \to \alpha \Rightarrow 0$

If α is large, 1st excited state is very much favored. And again, $C \sim 1/\alpha \Rightarrow 0$

Also, peak in C shifts to where 1 and $\alpha e^{-\beta\Delta}$ are comparable

Problem 7 Entropy-driven phase transition

i) G+T Prob 4.34

Sposed to use HardDisksMD program.

(a) Run simuln....
default params. Is T useful? (No) Does it fluctuate? (No!) Does P? ← yes

Answer No, T is not useful.... ∵ it rescales all velocities*, + is thus equivalent to changing timescale. Collisions are elastic, so disks don't swap energy. T is const thru simuln. On other hand, P does fluctuate.

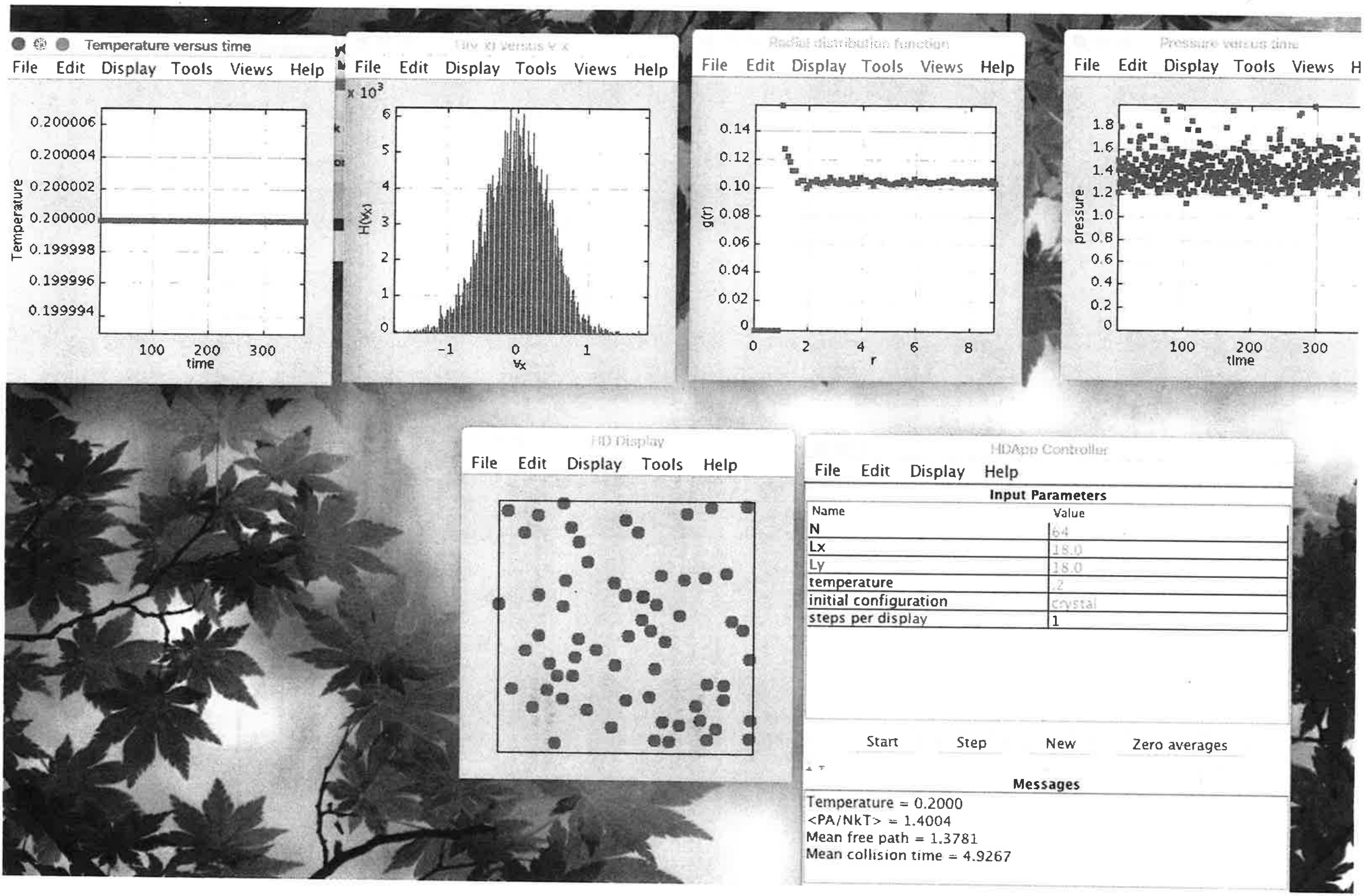
*which yeah, you can see in histogram of V_x

(b) Calculate PA/NkT. Phase transition perhaps, where P vs. N/A changes abruptly? (N/A is density in 2D)

Solution. Table S4.7 lists some sample data for $N = 64$ and $T = 1$. Near $\rho = 0.9$ there seems to be a sharp change in the pressure with a small change in density. It is known that there is a phase transition between a fluid and solid near this density. To simulate a crystal in two dimensions the lattice shape would need to be appropriate for a hexagonal lattice so that $L_y = (\sqrt{3}/2)L_x$. For $L_x = 8.2$ and $L_y = (\sqrt{3}/2)(8.2) = 7.1$ we have $\rho = 1.1$ and find $PA/NkT \approx 41$ and the system maintains its crystalline hexagonal lattice configuration, indicating that the system is well within the crystalline phase. For $\rho = 0.9$ with $L_x = 9.06$ and $L_y = 7.85$, we find $PA/NkT \approx 9.4$. At this density the crystal configurations are barely discernible, and the system is near the transition.

$L_x = L_y$	$A = L_xL_y$	density ρ	PA/NkT
18	324	0.20	1.40
16	256	0.25	1.56
14	196	0.33	1.82
12	144	0.44	2.42
10	100	0.64	4.16
9	81	0.79	7.32
8.5	72.25	0.89	10.8
8.2	67.24	0.95	16.0

Table S4.7: Results of Program **HardDisksMD** for a system of $N = 64$ hard disks.


Temperature versus time
File Edit Display Tools Views Help
Temperature
0.200006
0.200004
0.200002
0.200000
0.199998
0.199996
0.199994
100 200 300
time
File Edit Display Tools Views Help
x 10^3
H(vx)
0 1 2 3 4 5 6
-1 0 1
vx
File Edit Display Tools Views Help
g(r)
0 0.02 0.04 0.06 0.08 0.10 0.12 0.14
0 2 4 6 8
r
File Edit Display Tools Views H
pressure
0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8
100 200 300
time
File Edit Display Tools Help
HDApp Controller
File Edit Display Help
Input Parameters
Name Value
N 64
Lx 18.0
Ly 18.0
temperature .2
initial configuration crystal
steps per display 1
Start Step New Zero averages
Messages
Temperature = 0.2000
<PA/NkT> = 1.4004
Mean free path = 1.3781
Mean collision time = 4.9267

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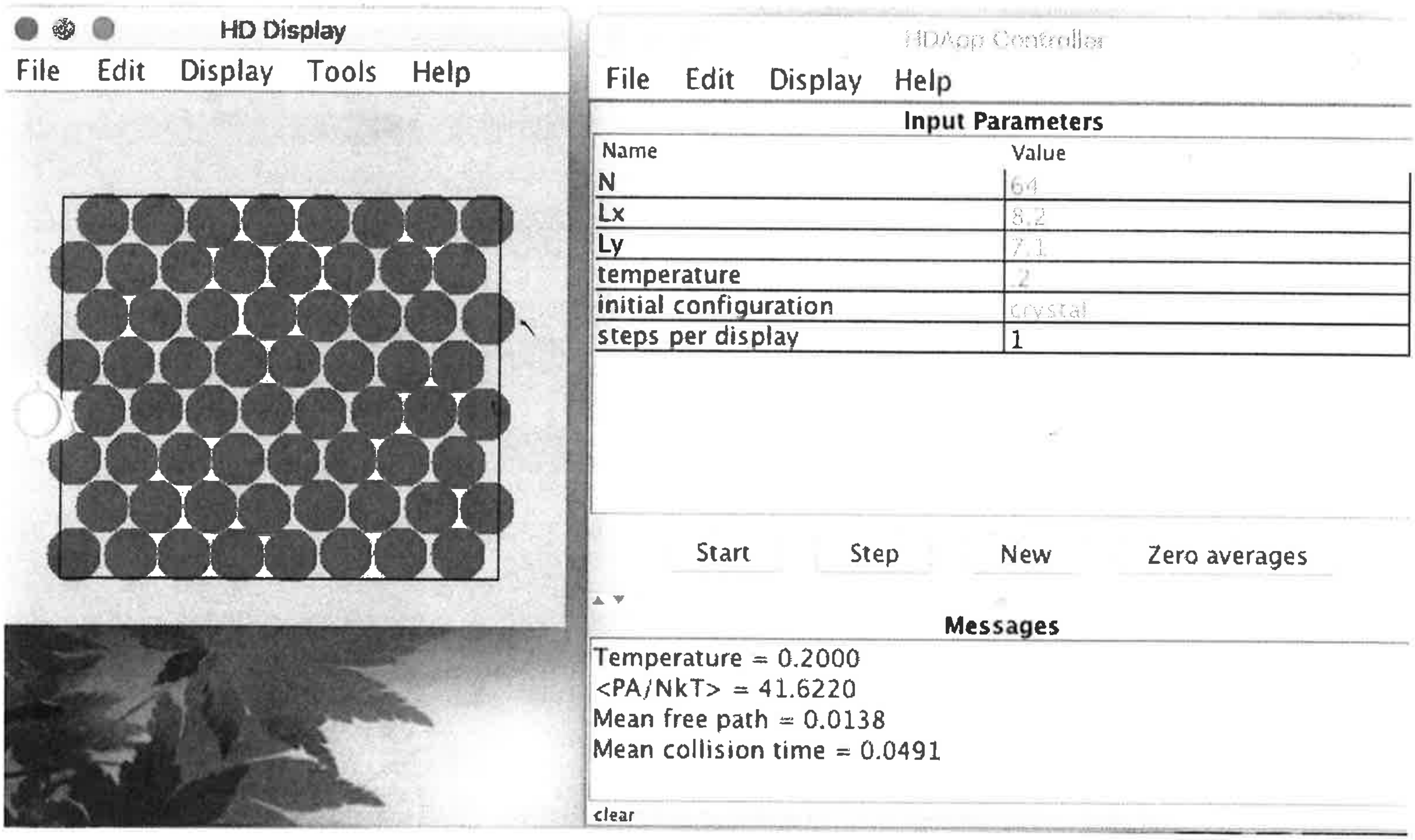
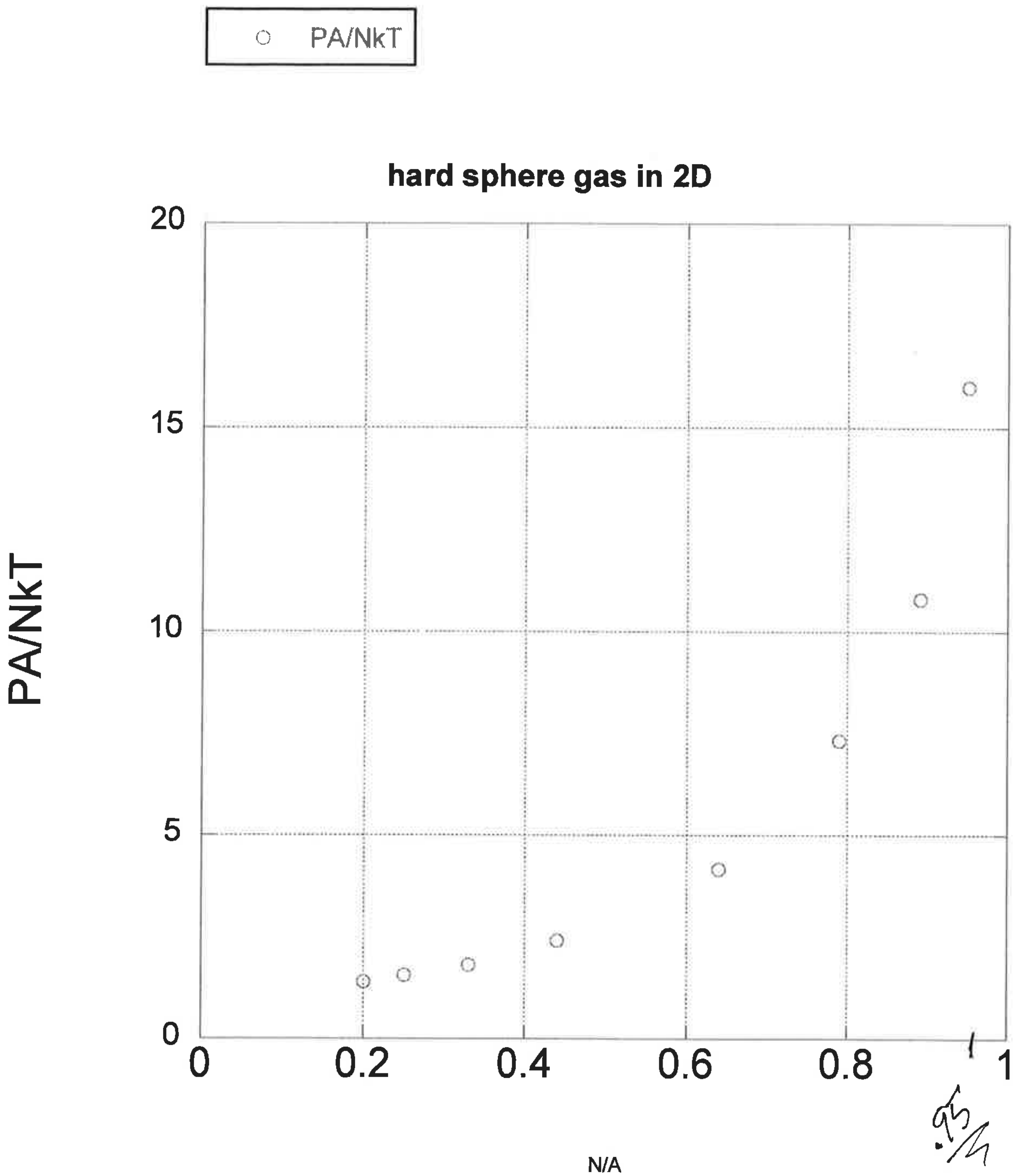

HD Display
File Edit Display Tools Help
HDApp Controller
File Edit Display Help
Input Parameters
Name Value
N 64
Lx 8.2
Ly 7.1
temperature .2
initial configuration crystal
steps per display 1
Start Step New Zero averages
Messages
Temperature = 0.2000
<PA/NkT> = 41.6220
Mean free path = 0.0138
Mean collision time = 0.0491
clear


PA/NkT
hard sphere gas in 2D
20
15
10
5
0
PA/NkT
0
0.2
0.4
0.6
0.8
1
.95/4
N/A

Hard discs

N=64 discs

$L_x = L_y$	$A = L_x L_y$	f	PA/NkT
18	324	.20	1.40
16	256	.25	1.56
14	196	.33	1.82
12	144	.44	2.42
10	100	.64	4.16
9	81	.79	7.32
8.5	72.25	.89	10.8
* 8.2	67.24	.95	16.0

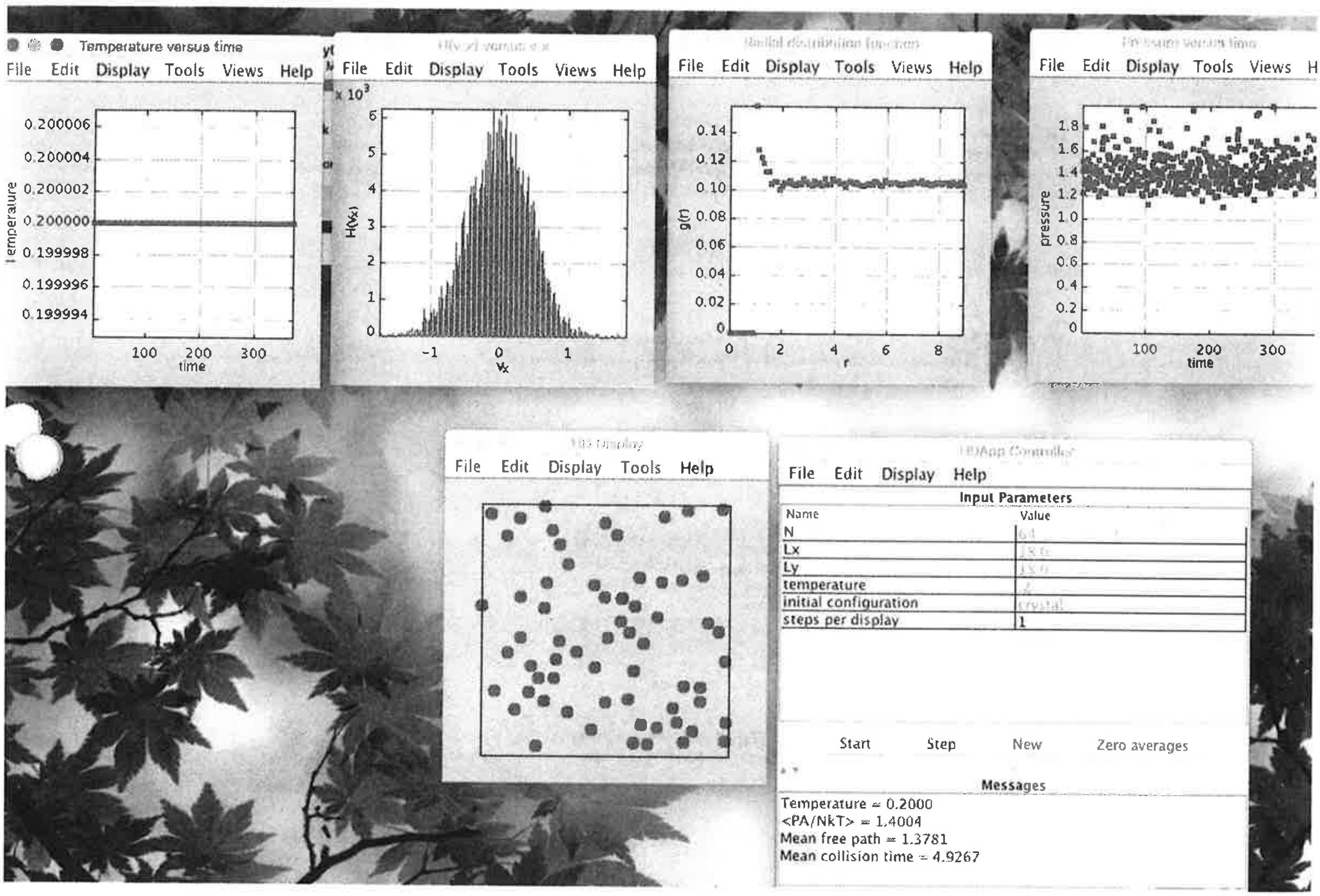
* Hexagonal crystal needs

$$L_y = \frac{\sqrt{3}}{2} L_x$$

$L_x = 8.2$ + $L_y = 7.1$

$\rho = 1.1$ + $PA/NkT = 41!$

Magic value is $\frac{\pi}{2\sqrt{3}} \simeq 0.9069$


Temperature versus time
File Edit Display Tools Views Help
temperature
0.200006
0.200004
0.200002
0.200000
0.199998
0.199996
0.199994
100 200 300
time
File Edit Display Tools Views Help
x 10^3
H(Vx)
Vx
File Edit Display Tools Views Help
g(r)
r
File Edit Display Tools Views H
pressure
time
File Edit Display Tools Help
File Edit Display Help
Input Parameters
Name
Value
N
Lx
Ly
temperature
initial configuration
steps per display
1
Start
Step
New
Zero averages
Messages
Temperature = 0.2000
<PA/NkT> = 1.4004
Mean free path = 1.3781
Mean collision time = 4.9267

7ii)

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Problem 4.56. The following demonstration illustrates an entropy-driven transition. Get a bag of M & Ms or similar disk-shaped candy. Ball bearings work better, but they are not as tasty. You will also need a flat bottom glass dish (preferably square) that fits on an overhead projector.

Place the glass dish on the overhead projector and add a few of the candies. Shake the dish gently from side to side to simulate the effects of temperature. You should observe a two-dimensional model of a gas. Gradually add more candies while continuing to shake the dish. As the density is increased further, you will begin to notice clusters of hexagonal crystals.

(a) At what density do large clusters of hexagonal crystals begin to appear?

Solution. If we use the diameter of the disks as the unit of length, then at a number density of $\rho \approx 0.9$, there is a transition from a fluid to a solid. You will see small solid-like clusters at lower densities. Larger clusters appear as ρ approaches 0.9.

(b) Do these clusters disappear if you shake the dish faster?

Solution. Shaking the dish faster does not eliminate the clusters. Instead the processes of cluster formation and cluster break up will occur faster.

(c) Is energy conserved in this system? Do the particles move if you do not shake the dish?

Solution. The disks will stop moving if you stop shaking the dish because of inelastic collisions between the disks and inelastic collisions of the disks with the walls of the dish.

(d) Compare the behavior of this system (an example of granular matter) to the behavior of a usual gas or liquid.

Solution. Because there is no attractive potential between the disks, there is no transition between a liquid and a gas. Also, because the interactions for these macroscopic disks is inelastic, energy is lost at each collision and must be supplied externally by shaking the disk. The lack of energy conservation leads to a velocity distribution that is not a Gaussian.

Problem 8

8: Fluctuations and No fluctuations:

i) **Fluctuations in a mole of gas** What is the probability that a mole of ideal gas at temperature T will have an energy that differs by a factor of 10^{-6} (i.e. one part in a million) from its mean energy?
Hint: Section 4.14.2 of G&T

In Section 4.14.2 of G+T we see a derivation leading to, in the Canonical distribution:

$$p(E) = p(\hat{E})\, e^{-(E-\hat{E})^2/2kT^2C_V}$$

This is a Gaussian, with

$$\sigma_E^2 = kT^2 C_V$$

For a mole of ideal gas, $C_V = \frac{3}{2}R$ *

* or $5/2$ if diatomic... doesn't matter.

$$\therefore \sigma_E^2 = \left(1.38\times10^{-23}\right)\frac{J}{K}(300\,K)^2\,\frac{3}{2}(8.3)\frac{J}{K}$$

$$\sigma_E^2 = 1.546\times10^{-17}\,J^2$$

and $\tilde{E} = \frac{3}{2}RT = 3735\,J$

Hence the probability of such a fluctuation, when compared with the probability of the mean, is

$$e^{-\Delta E^2/2\sigma_E^2} = e^{-\frac{(10^{-6})^2\tilde{E}^2}{2\sigma_E^2}}$$

$$= e^{-2.26\times10^{11}}$$

This is extremely small!

NB Could have also found $p(\tilde{E})$ by properly normalizing gaussian.... it is.

$$P(\hat{E}) = \frac{1}{\sqrt{2\pi\sigma_E^2}}$$

$$P(\tilde{E}) = \frac{1}{\sqrt{2\pi k T^2 C_V}} \doteq 1.014 \times 10^{8}$$

But this is just a weight to normalize gaussian ...
it is relative prob. that counts ..
+ fact that over 99% of time,
E is within $3\sigma_E$ of mean

where $\dfrac{\sigma_E}{\bar{E}} = 1.05272 \times 10^{-12}$

So one part in 10^{12} .... ☺