SUMMARY SHEET

EXPERIMENT 2

Is the total momentum conserved? YES /~~NO~~

Accuracy of computer calculation $100\frac{0.0000018}{0.1} \approx 0.002\%$ 0:1

(RMS velocity = 0.1)

Time	Total Energy
0	-1.61499
2	-1.62886
4	-1.62878
6	-1.62301
12	-1.62882
18	-1.62599
24	-1.62796
30	-1.62703
50	-1.62753
70	-1.62676
90	-1.62580
130	-1.62713
180	-1.62409

Does the system conserve energy? YES/~~NO~~ (~ ±1%)

Equilibrium value of E_k* (Average 24 to 180) = 0.534 ±0.05

Equilibrium time SD (see Fig. E 2.1) ≅ (10 to 20)×0.1

Value of *S* recorded > 20, e.g. 60

Value of α (for *SD*=60) (see Fig. E2.2) = 0.503

Accuracy of α = ±0.02

For what time number range is graph, obtained using first value of *SR*, linear? *SZ* = 18 to 24

Gradient of this graph in linear region	≅ 0.027 to 0.47
Accuracy of gradient	= 0.002
Gradient of AVERAGE $<R^2>$ in linear region	= 0.035
Accuracy of this gradient	= ± 0.01

* delete as appropriate

Is the system a liquid/solid? Liquid/~~Solid~~*

Mean Momentum of the system at requested steps (*S*)

S	*<VX,1>*	*<VY,1>*	*<PX>*	*<PY>*
0	0.0000000	0.0000000	0.000000	0.000000
40	0.0000010	0.0000016	0.000048	0.000077
80	0.0000018	0.0000001	0.000086	0.000005
120	0.0000014	0.0000007	0.000067	0.000034
160	0.0000016	0.0000010	0.000077	0.000048

Energy of the system at requested steps (*S*)

S	*<VX,2>*	*<VY,2>*	*<KE> = T**	*<U>*	*<E>*= Total Energy
0	0.0173874	0.0142851	0.760140	-4.7502660	-1.61499
2	0.0162506	0.0131025	0.704474	-4.6666675	-1.62886
4	0.0124966	0.0089562	0.514867	-4.2873015	-1.62878
6	0.0077405	0.0039113	0.279643	-3.8053113	-1.62301
12	0.0118740	0.0120959	0.575278	-4.4081878	-1.62882
18	0.0099579	0.0075854	0.421039	-4.0940627	-1.62599
24	0.0108577	0.0116978	0.541332	-4.3385782	-1.62796
30	0.0126065	01000340	0.543372	-4.3407997	-1.62703
50	0.0127138	0.0103334	0.553133	-4.3613165	-1.62753
70	0.0088657	0.0158292	0.592678	-4.4388669	-1.62676
90	0.0107740	0.0076446	0.442087	-4.1357699	-1.62580
130	0.0073008	0.0177446	0.601090	-4.4564333	-1.62713
180	0.0097161	0.0096426	0.464609	-4.1773882	-1.62409

All values are in reduced units. <*KE*> is the mean kinetic energy per atom. <*U**> is twice the potential energy. <*VX*,2> and <*VY*,2> are the mean values of the squares of the *X* and *Y* velocity components, as described in the question. Similarly <*VX*,1> and <*VY*,1> are the mean values of the velocity components. <*PX*> and <*PY*> are the mean momentum per particle.

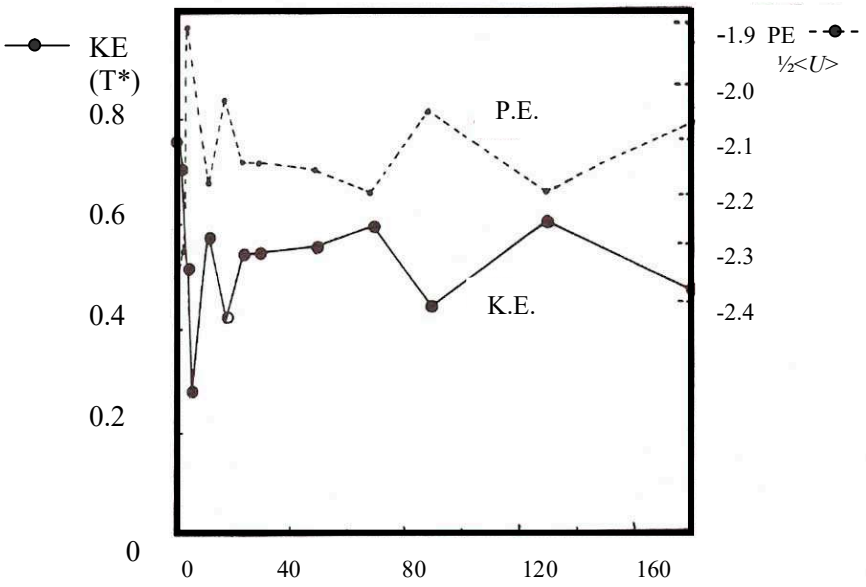


Figure E 2.1

Variation of K.E and P.E.

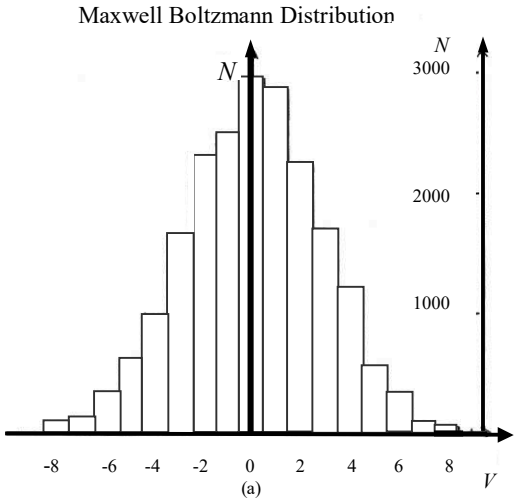
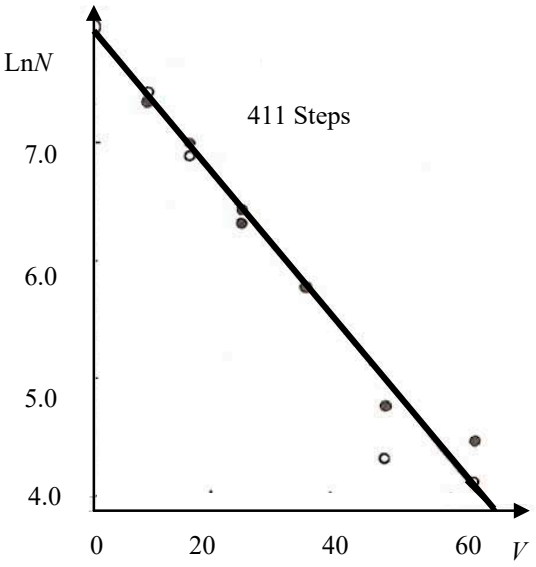
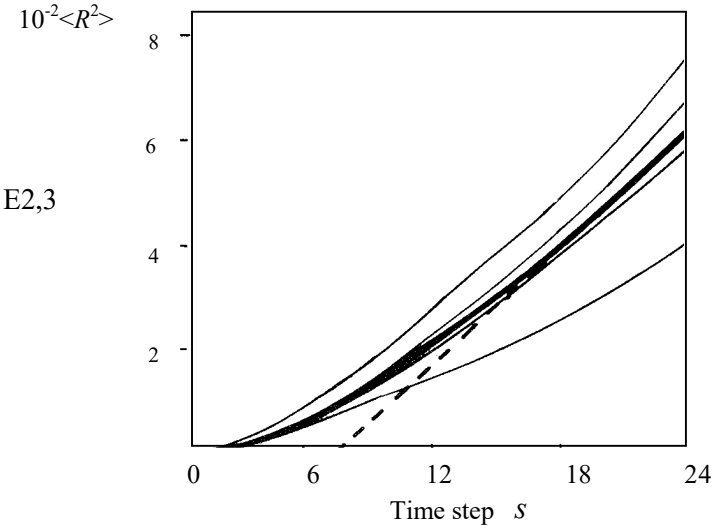


Figure E2.2



(b)

Figure E2,3



$<R^z>$ curves as a function of time

TYPICAL RESULTS : NOTE THE LARGE VARIATIONS IN THE VALUES OF $<R^2>$

Time Number SZ - S-SR	SR = 261 $<R^2>$	SR = 301 $<R^2>$	SR = 334 $<R^2>$	SR = 370 $<R^2>$	AVERAGE $<R^2>$
0	0	0	0	0	0
2	0.00088	0.00067	0.00091	0.00079	0.00081
4	0.00287	0.00276	0.00382	0.00298	0.00311
6	0.00523	0.00628	0.00858	0.00623	0.00658
8	0.00797	0.01101	0.01449	0.01039	0.01097
10	0.01143	0.01656	0.02095	0.01523	0.01604
12	0.01528	0.02235	0.02768	0.02022	0.02138
14	0.01874	0.02845	0.03453	0.02564	0.02684
16	0.02184	0.03539	0.04157	0.03160	0.03260
18	0.02526	0.04293	0.04902	0.03833	0.03889
20	0.02979	0.05080	0.05718	0.04532	0.04577
22	0.03538	0.05918	0.06605	0.0510	0.05303
24	0.04063	0.06784	0.07533	0.05569	0.05987