

Vu-Linh Nguyen - 2256347

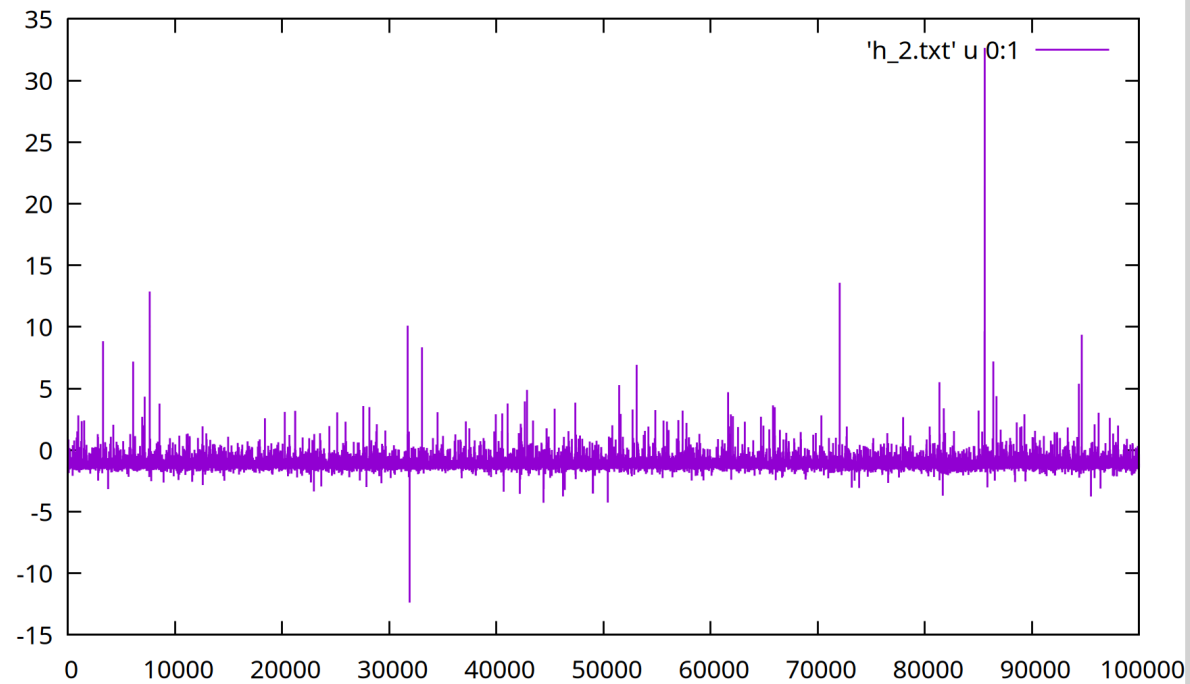
Computational Condensed Matter Physics - Makeup exam

A.2

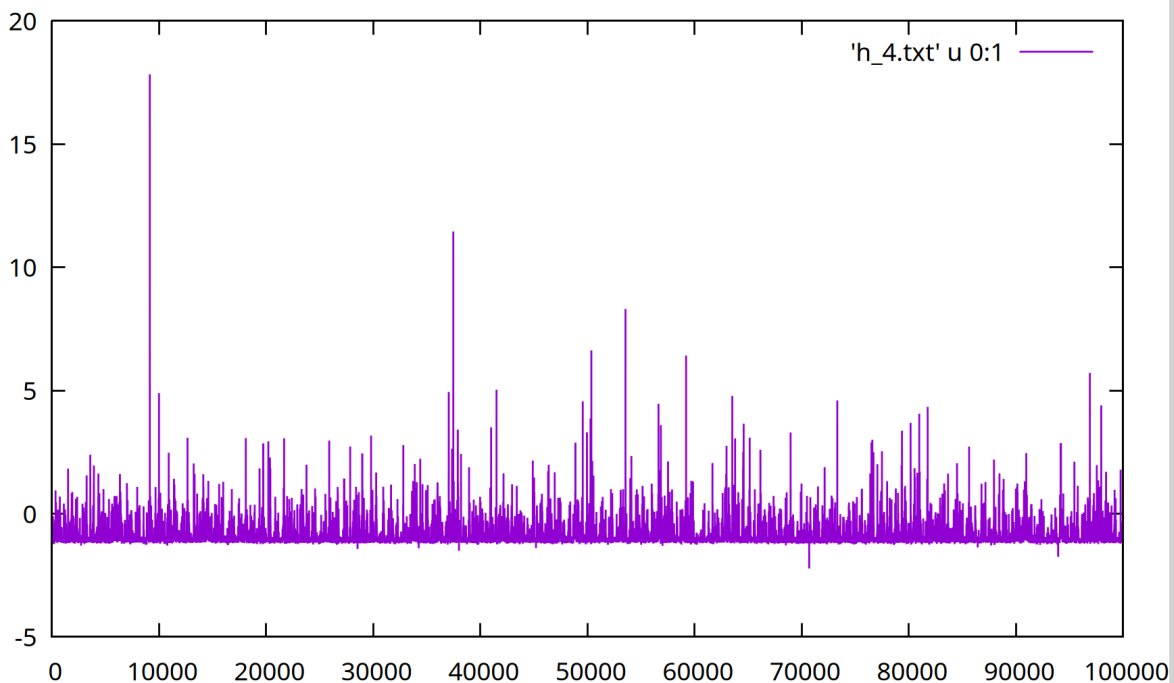
B = 1

I take the limit of A and F to be small for my code $A=F^2=.0005$

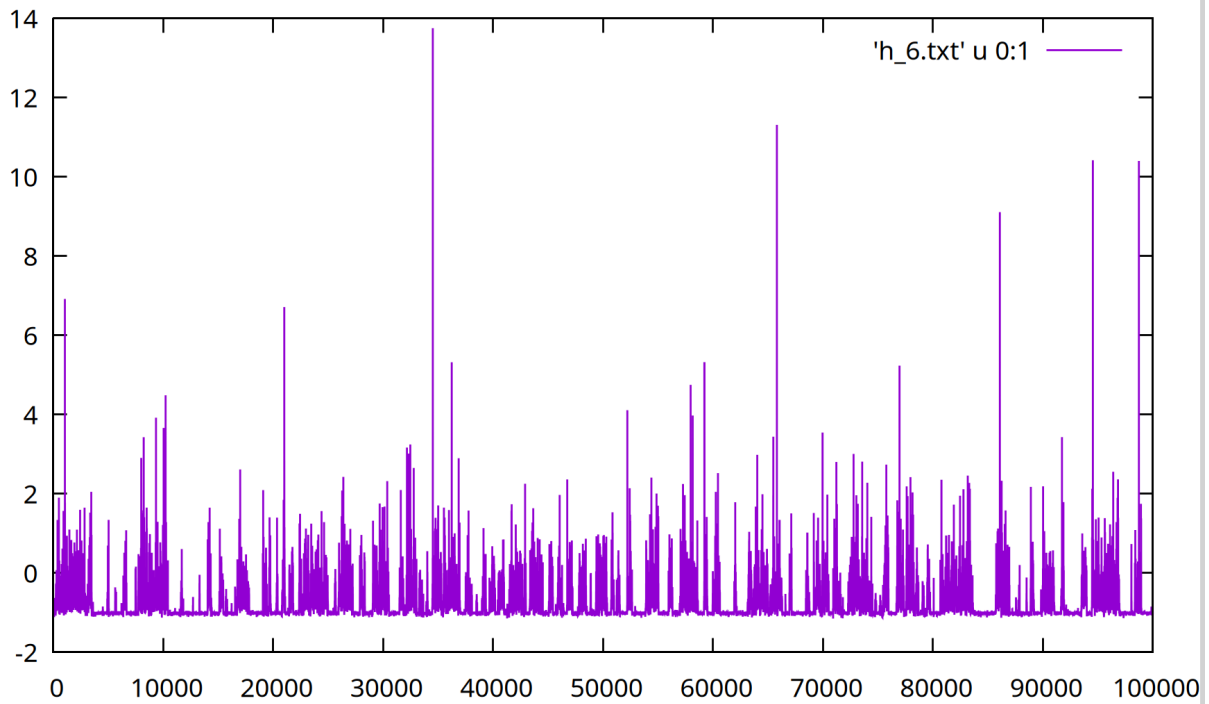
The local energy versus step, for $d=2$, we don't need to remove any data



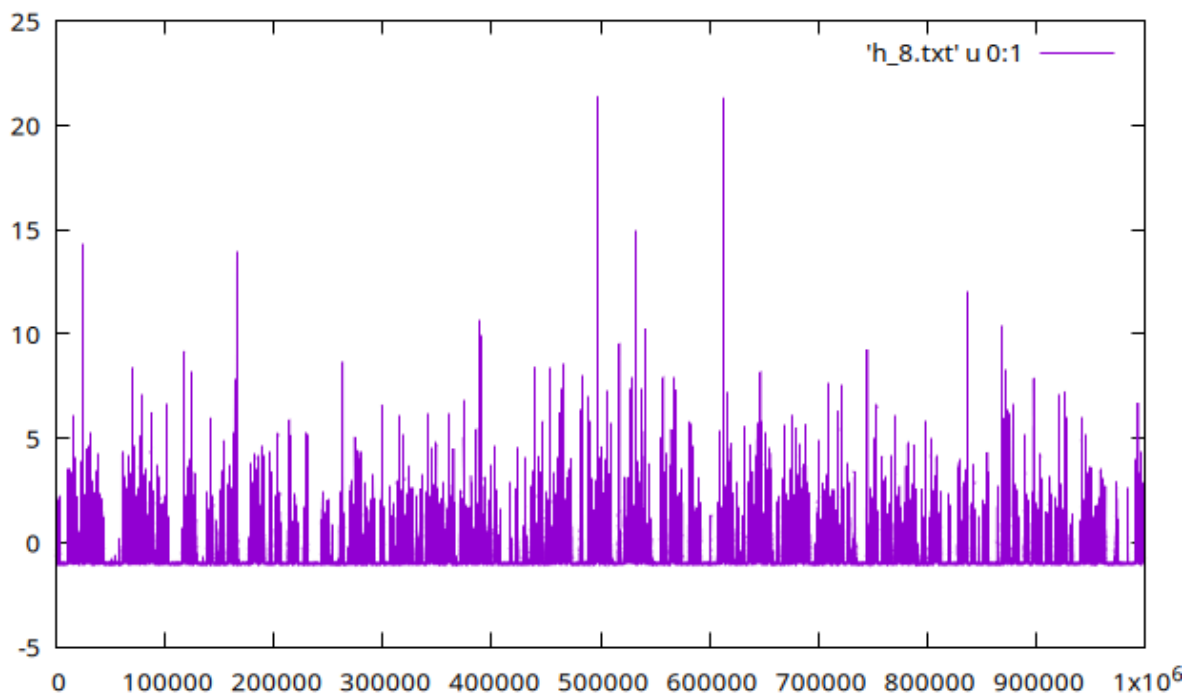
The local energy versus step, for $d=4$, we don't need to remove any data



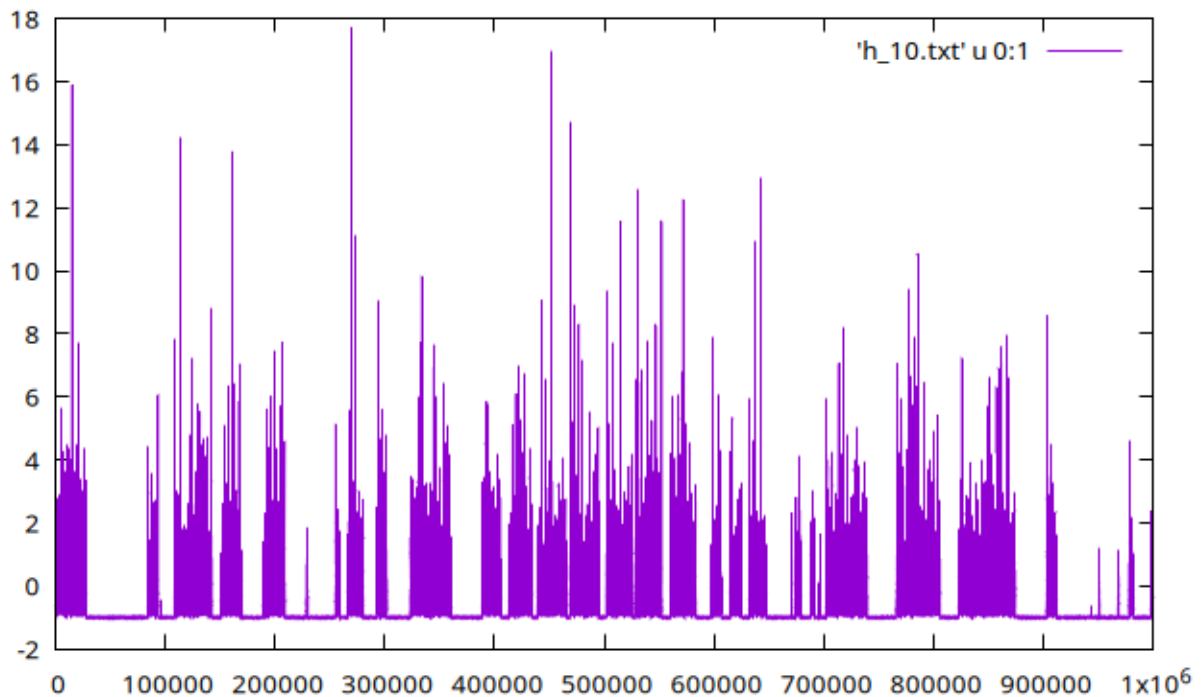
The local energy versus step, for $d=6$, we don't need to remove any data



The local energy versus step, for $d=8$, we don't need to remove any data, however, I need to increase the number of steps up to $1e6$ to sample



The local energy versus step, for $d=10$, we don't need to remove any data, however, I need to increase the number of steps up to $1e6$ to sample



Summary we have the table

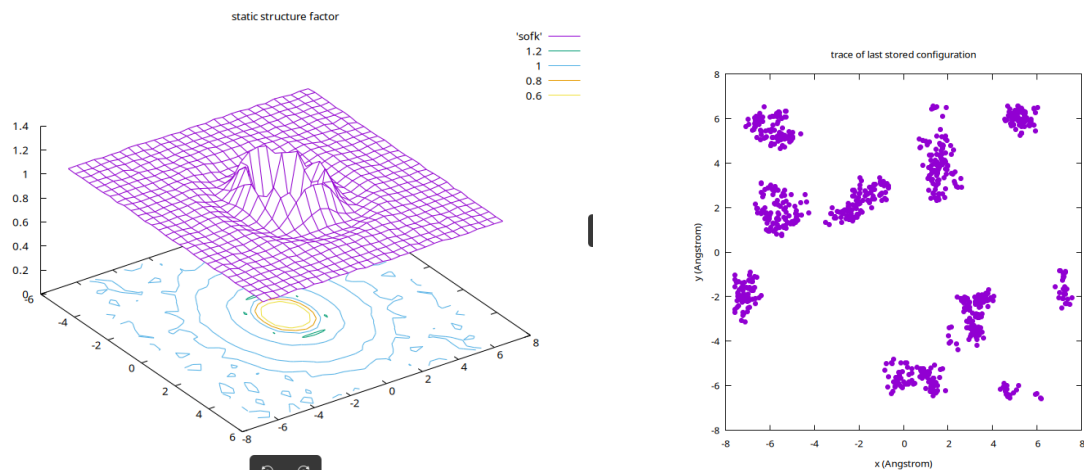
d	size of the move	Acceptance rate	Energy	Exam energy	Absolute difference
2.0	2	0.489(1)	-1.079(4)	-1.0808(14)	0.0018(42)
4.0	2	0.477(2)	-0.896(7)	-0.8946(15)	0.0014(70)
6.0	2	0.451(2)	-0.79(1)	-0.7931(17)	0.0031(150)
8.0 (1e5)	2	0.439(2)	-0.804(15)	-0.7558(18)	0.0482(15)
8.0 (1e6)	2	0.4389(5)	-0.754(5)	-0.7558(18)	0.0018(53)
10.0 (1e6)	2	0.436(5)	-0.733(5)	-0.7395(17)	0.0065(52)

For the large d, two hydrogen nuclei are far away from each other, it might make of configuration space is larger, it means we do need to sample the larger number of steps to have the reasonable accuracy.

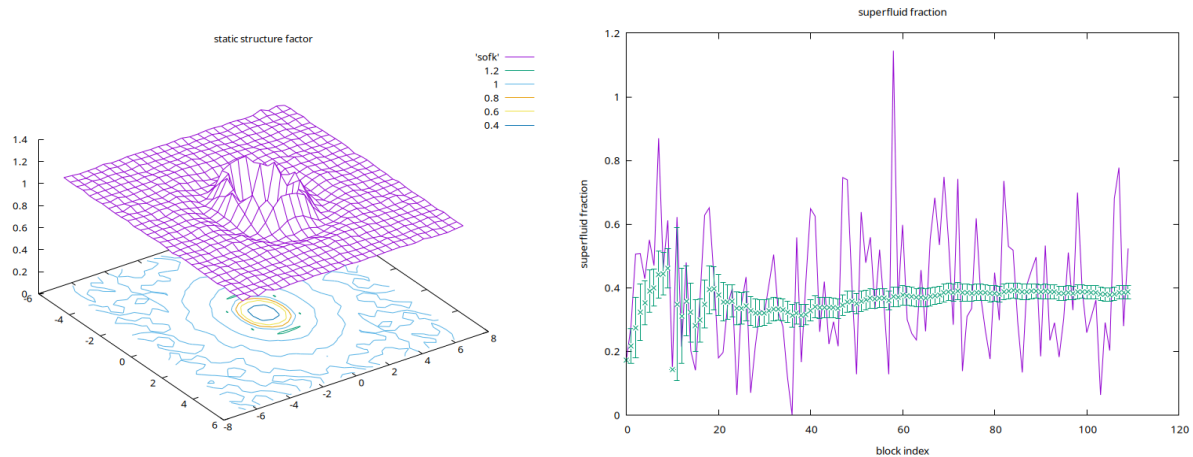
A.3 The best solution that I can think of is to change the large size of the move, but still have the reasonable acceptance rate with $\delta=2.5$, I got $E=-0.77(2)$ with the acceptance rate 0.341(2).

A.4 I need more time to set up the code but we can observe that this wave function has the symmetrical properties, I think this would make our calculation more efficient. Because VMC does depend on the wave function.

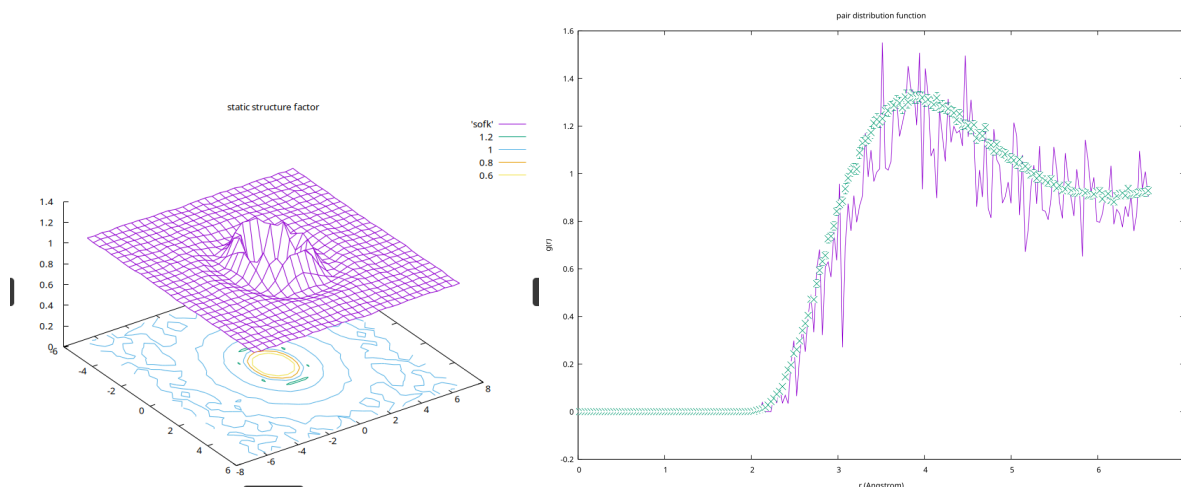
B.1 $T = 2.5$, $\text{ntau}=100$, this is liquid phase, you can see it from the structure factor



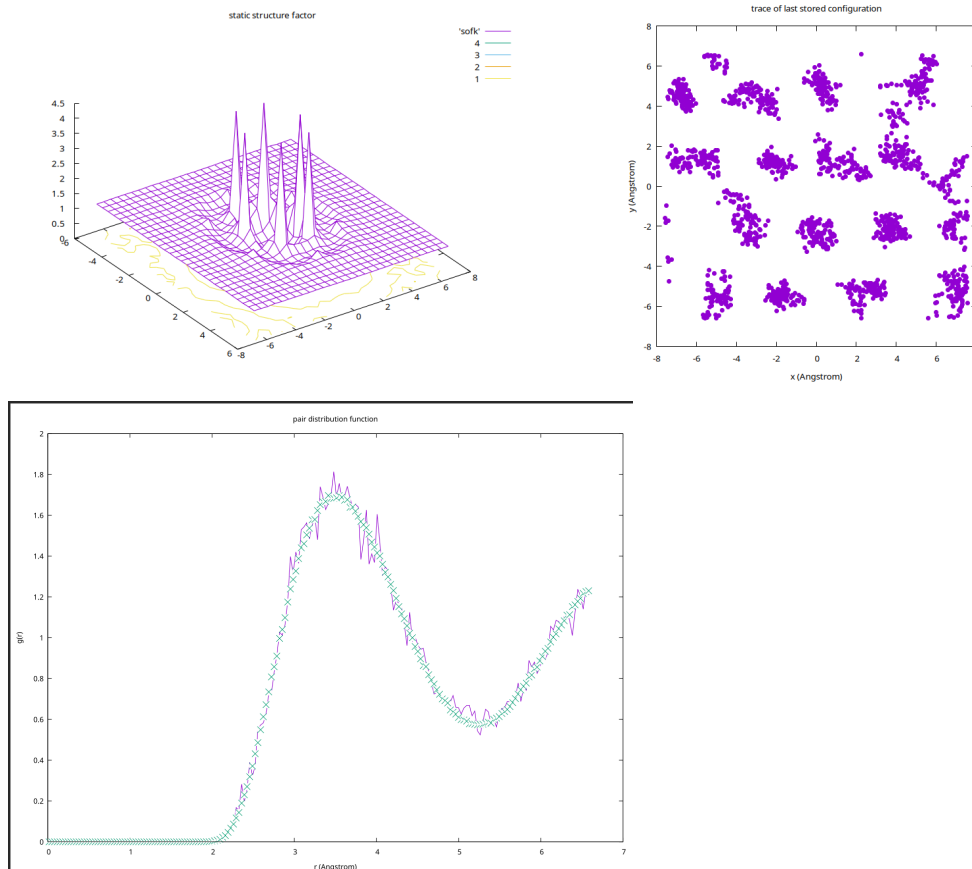
At $T=1K$, $\text{ntau}=200$, I get superfluid phase, $\rho_{\text{he}} = 0.385(21)$



B.2, with 2.5K, chemical potential 0.. At this temperature, I predict we can have superliquid phase transition, or solid phase transition. At first, I got the liquid phase with the superliquid fraction around 0.0143

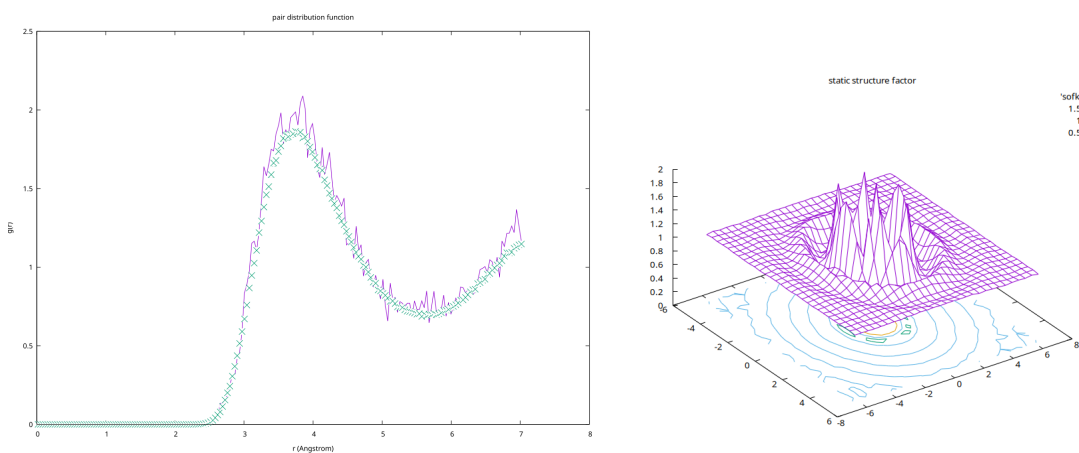


Now let's increase the chemical potential, we change mbar to 20, at $\mu=20$ to get around 0.5 wiggle, I get the crystal phase.

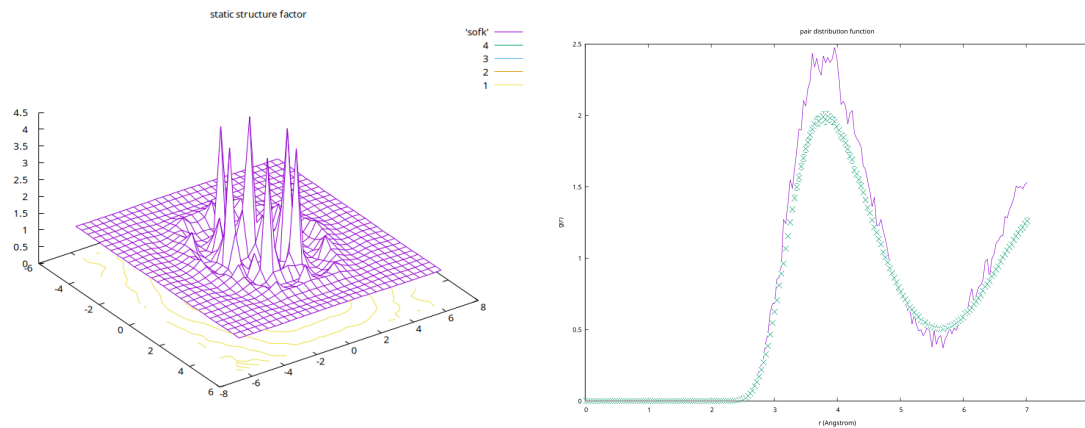


B.3 Now we change to the H system

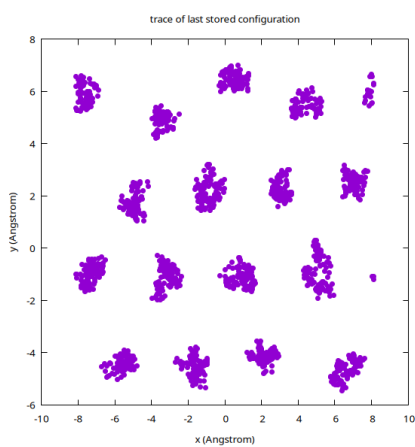
At $T=20\text{K}$, $\text{ntau}=50$, I got the liquid phase by looking at the $g(r)$ and structure factor, we have the peak due to we have rough estimation on our calculation, but we have circle structure factor \rightarrow liquid,



I change the $T=10\text{K}$, and $\text{ntau}=100$, to keep the sample epsilon, I got many Bragg peak \rightarrow solid phase.



I have around 15 number of particles inside the simulation box, the particles quite move wiggle around their positions and we can see the clear pattern.



B.5 The difference between B1 and B3 is we don't get the superfluid phase in H₂, and we don't the solid phase of He when we reduce the temperature.

B.4

I change mbar to 20 to adjust the wiggle around 0.5 for the h2 input file. I adjust the μ up to 30 but still can not see the phase transition. At $\mu=50$ I got the solid phase

