

## Quantum Monte Carlo test: answers

### Part A

1. Why do we use correlated wave functions such as (2) and (3)?

To improve the accuracy of the variational description of the system (as seen, for instance, from the reduction of the fluctuations of the local energy as one includes two-body, three-body and backflow correlations in the trial function),

2. Why do we use Monte Carlo to calculate expectation values with wave functions such as (2) and (3)?

Because these expectation values are integrals in a highly dimensional space.

3. How do we choose the time step (size of the move) in VMC?

By minimizing, for a given number of Monte Carlo steps, the statistical error (or, more quickly, by arranging for an acceptance rate not too far from 50%).

4. Does the average energy depend on the time step in VMC?

No. Only the efficiency depends on the time step.

5. How do we choose the time step and the trial energy in DMC?

The time step should be small enough to guarantee a good approximation to the propagation in imaginary time. Typically one starts with  $\sim 1/10$  of the time step used in VMC and, in principle, extrapolates to time step zero.

6. Does the average energy depend on the time step in DMC?

Yes. Each step in the imaginary time evolution samples an approximation to the propagator which becomes exact in the limit of zero time step.

7. Why do we need a population of walkers in DMC?

The propagator is the product of a factor which is sampled directly and a weight. In order to reduce the fluctuations, the weight is transformed into multiplicity in the branching algorithm, which requires a population of walkers.

8. Does the average energy depend on the number of walkers in DMC?

Yes. The number of walkers fluctuates, and it must be controlled by deleting walkers when they are too many or replicating walkers when they are too few. This introduces a bias which vanishes when the average number of walkers is infinite.

9. For a potential which diverges at zero distance, do spin-1/2 fermions have a different cusp condition in the Jastrow factor for parallel or antiparallel spins?

Yes. Parallel spins have a contribution to the cusp from the determinant.

10. Does the cusp condition apply to bosons? If the parallel and antiparallel fermion cusp conditions are different, which one applies to bosons?

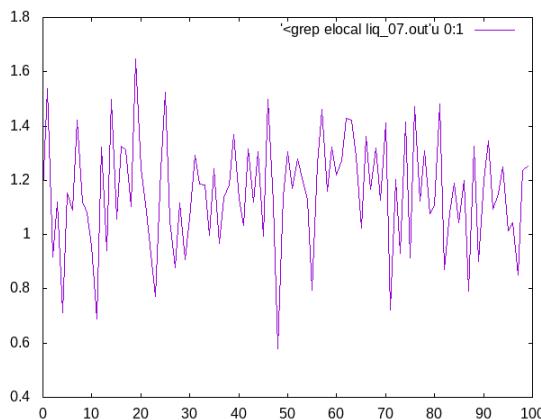
Yes. For bosons we use the same cusp condition as for antiparallel spin fermions, which is not affected by the determinant.

## Part B

1. I used an input file with the line “vmc 100 1000 0.01 0”, which for density 0.07 gives (from the output files, with the statistical error on the last two digits in parentheses):

	acc. rate	e <sub>local</sub>	e <sub>2</sub>
liquid	0.4626(13)	1.155(21)	10.41(45)
solid	0.5805(12)	1.010(10)	3.97(17)

There is no need of discarding initial blocks for equilibration, see e.g the plot of the block averages for the liquid phase:

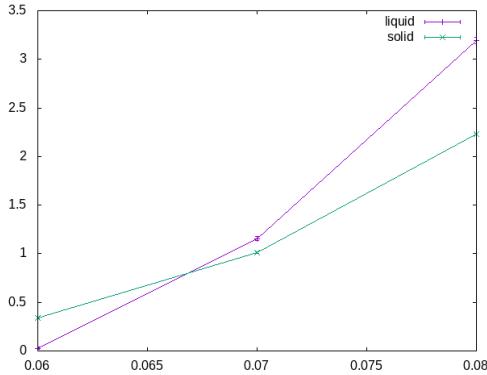


The acceptance rate is somewhat different for the two phases, but acceptable in both cases.

The analysis with statfor.f gives “t corr = 1” in both cases, which means that the block averages are statistically independent and the statistical errors from the output files are reliable.

The variance of the local energy is e<sub>2</sub> minus the square of e<sub>local</sub>: 9.1 for the liquid and 2.9 for the solid. Guided by the zero variance property of the local energy, we can say that at this density the Nosanow wave function is more accurate for the solid than the Jastrow wave function is for the liquid.

2. I made 4 more simulations: liquid and solid for densities 0.06 and 0.08. I changed the time step to 0.012 and 0.008 at these two densities, respectively (however, using the same time step 0.01 as in question 1 is acceptable). The result is shown in this figure:



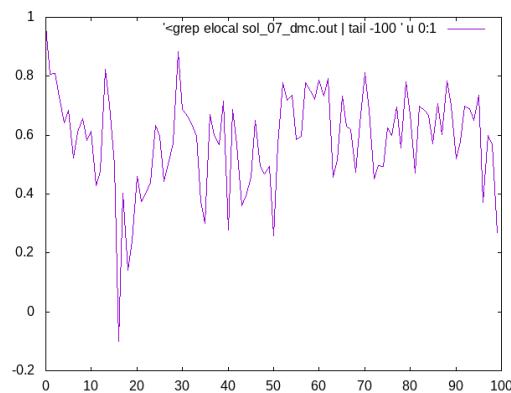
which shows that the crystallization density is  $\sim 0.067$ .

3. For the DMC simulations at 0.07, for each phase, I first run a short VMC run to save 50 configurations as the initial population of walkers using the input line “vmc 10 1000 0.01 200”

Then I run the DMC simulation with the input line  
“dmc 100 100 0.001 50 1.0”

i.e. taking a time step 10 times smaller than in VMC and a trial energy 1.0 which is close to the variational energy of question 1 (for both phases).

The plot of the block averages for the solid phase is as follows:



On this plot, the first  $\sim 10$  blocks are consistent with a decrease of the energy from the variational result ( $\sim 1.0$ ) to a fluctuating behavior around a lower, stationary value. Therefore, I calculate the average energy only on the last 90 blocks with statforw.f:  
“grep elocal sol\_07\_dmc.out | tail -90 | awk ‘{print \$1, \$4}’ | ./statforw”  
(where sol\_07\_dmc.out is my output file). The correlation time “t corr” is 3.6, which shows that the block averages are not statistically independent and the statistical error in the output file is underestimated.

Note that these results on equilibration and correlation time may depend on the number of steps per block of your run, so you may have found different results. One can also eliminate equilibration blocks with a preliminary short equilibration run. All that matters is that your final energy and statistical error comes from a correct analysis of your output file.

The VMC and DMC results of the liquid and solid phases at this density are:

	VMC	DMC	difference
liquid	1.155(21)	0.376(28)	0.779(35)
solid	1.010(10)	0.570(34)	0.440(35)

One can see that the DMC simulation lowers the energy of the liquid more than that of the solid. Therefore, DMC would shift the crystallization density to a higher value.

The error in the variational energy (the difference in the last column) is smaller for the solid than for the liquid. This is consistent with the observation on the quality of the wave functions of question 1 based on the variance of the local energy.