

This test is divided in two parts, each worth up to 40 points (i.e. to get the maximum grade it is sufficient to complete correctly 3/4 of either part).

A. For the part on the **Hydrogen molecule**, you will use your own code to calculate the variational energy for this Hamiltonian

$$H = -\frac{1}{2} \sum_i \nabla_i^2 - \sum_{i,j} \frac{1}{|\mathbf{r}_i - \mathbf{d}_j|} + \frac{1}{r_{12}} + \frac{1}{d}$$

starting with this wave function

$$\Psi = \phi(\mathbf{r}_1)\phi(\mathbf{r}_2); \quad \phi(\mathbf{r}) = e^{-\beta|\mathbf{r}-\mathbf{d}_1|} + e^{-\beta|\mathbf{r}-\mathbf{d}_2|},$$

with $d = |\mathbf{d}_1 - \mathbf{d}_2|$, i.e. *without the Jastrow factor* (you can keep it in your code and set A and F to very small values).

B. For the part on **Path Integral Monte Carlo** for ${}^4\text{He}$ and H_2 , you will use the code `worm.f` included in this folder. Both Helium atoms and Hydrogen molecules are described as zero-spin point-like particles interacting via a Lennard-Jones potential, $v(r) = 4\epsilon[(\sigma/r)^{12} - (\sigma/r)^6]$. For Helium, $\epsilon = 10.22\text{K}$ and $\sigma = 2.556\text{\AA}$; for molecular Hydrogen, $\epsilon = 36.7\text{K}$ and $\sigma = 2.96\text{\AA}$.

Note that the code `worm.f` is **NOT** the same as in lab3 or in the midterm test. Also, the `worm README` included in this folder describes an updated feature "restart -1".

The files `statfor.f` and `statforw.f` for the statistical analysis included in this folder are the same as in lab1,2,3.

Assignments

For each question, write the answer on a text file and keep a copy of the relevant output file(s) (for part B, it is advised to save the output files in a separated subfolder for each run, to prevent overwriting).

Note that you may or may not include files with your plots, as you prefer, as soon as the relevant data are available: for instance, you can just type "I see Bragg peaks in $S(k)$, data in file subfolder_xxx/sofk".

At the end of the test, compress the folder with your work and send it by email to saveriomoroni@gmail.com.

Part A. Hydrogen molecule

1. Put a copy of your code in the folder of your exam
2. Set the variational parameter to $\beta = 1$, adjust the size of the move δ to get an acceptance rate of about 50%, and compare your variational energy E for a few values of the distance d with the following table:

d	2.0	4.0	6.0	8.0	10.0
E	-1.0808(14)	-0.8946(15)	-0.7931(17)	-0.7558(18)	-0.7395(17)

Show that for large d you face ergodicity issues (e.g. dependence on the initial configuration, and/or inconsistent results, and/or trace of a quantity such as the local energy or the coordinate along the axis of the molecule...).

3. Modify the move to overcome the ergodicity issues.

Hint: in order of increasing efficiency and complexity (and score) you can (i) change δ , (ii) change the geometry of the move, or (iii) devise and implement an additional move.

4. Modify the code to use the Heitler-London form wave function,

$$\Psi_{HL} = e^{-\beta|\mathbf{r}_1 - \mathbf{d}_1|} e^{-\beta|\mathbf{r}_2 - \mathbf{d}_2|} + e^{-\beta|\mathbf{r}_1 - \mathbf{d}_2|} e^{-\beta|\mathbf{r}_2 - \mathbf{d}_1|}.$$

Why it is more accurate than the starting Ψ , particularly for large d ?

Part B: Path Integral Monte Carlo

1. Copy the sample input file `worm.in_he` for ${}^4\text{He}$ into `worm.in`, compile and run the code `worm.f`, redirecting the standard output to `worm.out`. What is the phase of the system? Save the output files that describe the initial phase. Decrease the temperature, keeping the “time step” fixed, until you observe a phase transition. Save and comment the output files that describe the final phase.
2. Starting again from the sample input file for ${}^4\text{He}$, increase the density at fixed temperature until you observe a phase transition. Save and comment the output files that describe the final phase.
3. Copy the sample input file `worm.in_h2` for H_2 into `worm.in` and run the code. What is the phase of the system? Save the output files that describe the initial phase. Decrease the temperature, keeping the “time step” fixed, until you observe a phase transition. Save and comment the output files that describe the final phase.
4. Starting again from the sample input file for H_2 , increase the density at fixed temperature until you observe a phase transition. Save and comment the output files that describe the final phase.
5. Briefly discuss the differences found between the results of items 1 and 3.