

First intermediate test: quantum Monte Carlo

In this folder you find the following files:

- test.pdf: this file
- 2degas.pdf: Ref. [1] (in this paper, Diffusion Monte Carlo (DMC) is called Green's function Monte Carlo)
- setup.f: a setup fortran code
- qmc.f: a QMC fortran code
- qmc.h: a file included by qmc.f at compile time
- statfor.f: fortran code for averages and statistical errors
- statforw.f: fortran code for weighted averages and statistical errors

For documentation on the the setup and qmc codes, and recommended procedures to run specific simulations (VMC, optimization, DMC) refer to the file doc.pdf that you have already downloaded from the link “2degas” in the e-learning page of the course.

You should be familiar with the use of the codes statfor.f and statforw.f; if not, ask for instructions.

Compile all four fortran codes. With gfortran, you can use the option -w to suppress warning messages, option -O3 to get a faster executable, -o filename to choose the name of the executable, and -Wno-argument-mismatch (or -fallow-argument-mismatch) if you get argument mismatch errors.

You should have implemented a Variational Monte Carlo (VMC) code for the Helium atom with a trial function $\exp(-\beta r_1 - \beta r_2)$ (and possibly other trial functions). Create a subfolder and put a copy of your code(s) there.

Important note: You are not requested to answer all of the questions.

Assignments

For each question, write the answer on a text file and keep a copy of the relevant output files.

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

Part A. The Helium atom

- A1) The virial theorem states that $2 \langle T \rangle + \langle V \rangle = 0$ for stationary states (e.g. eigenstates of H or variational states with optimized variational parameters). Use the virial theorem to find the optimal value of the variational parameter β . A reasonable starting point is $\beta=2$, because it is the exact solution of the non-interacting problem. Why can we expect that the optimal value of β is somewhat smaller?
- A2) Modify the code to calculate the variance of the local energy; compare with the result provided by statfor. If the trial function does not fulfill the electron-nucleus and/or the electron-electron cusp condition, does (i) the local energy, (ii) the variance of the local energy, (iii) the variational energy diverge?
- A3) Modify the code to calculate the variational energy for a few (two or three) values of β with a single simulation using the reweighting method. What happens if you choose values of β too far from each other? (state in words and/or show with data).
- A4) Modify the code to calculate the Hellmann-Feynman force $\mathbf{F}_{\text{HF}} = - \langle \nabla_{\mathbf{S}} V \rangle$ (at least one cartesian component), where \mathbf{S} is the position of the He atom. The exact result is $\mathbf{F}_{\text{HF}}=0$ by symmetry. Repeat the simulation a few times: you should find an unexpected behavior, particularly for the statistical error. Can you identify (i) the unexpected behavior and (ii) its origin?
- A5) If you included further generalizations in you code (e.g. modification of input/output, calculation of averages, on the fly, better wave functions, first spin-singlet excited state, spin-triplet ground state, other...) add a brief statement of what it does and how to use it.

Part B. The spin-polarized 2D electron gas

- B1) Calculate the non-interacting energy at $r_s=1$ for a fully spin-polarized electron gas in two dimensions (i) in the thermodynamic limit and (ii) for $N=21$ electrons in a square box with periodic boundary conditions.
- B2) Choose one value of r_s in the set $\{5,10,20\}$. Introduce two- and three-body correlations and backflow for $N=21$ spin-polarized electrons and optimize the wave function. Run a VMC simulation with the optimized wave function for further reference.
- B3) Run a fixed-node DMC simulation for the same system as in B2). Do you expect/see a dependence of the DMC energy on (i) the time step and (ii) the number of walkers? Use the results of the simulations in B2) and B3) to calculate the extrapolated estimate of the kinetic energy.
- B4) Assume that eq. (19) of Ref. [1] holds for the DMC energy of the polarized electron gas with the values $b_1(r_s)$ and $b_2()$ given in Table III of Ref. [1]. Using data from B1) and B3), give an estimate of the DMC energy of the spin-polarized electron gas at your chosen value of r_s in the thermodynamic limit.
- B5) The Hartree-Fock energy for the 2D electron gas with density parameter r_s and spin polarization ζ in the thermodynamic limit is:
- $$\frac{1}{2r_s^2} [(1 + \zeta)^2 + (1 - \zeta)^2] - \frac{4\sqrt{2}}{3\pi r_s} [(1 + \zeta)^{3/2} + (1 - \zeta)^{3/2}] \quad (*)$$
- Using data from B4), calculate the correlation energy (under the assumption that the error of the fixed-node approximation is negligible). Compare with the correlation energy of Table III of Ref. [1]: are correlations stronger for $\zeta=0$ or $\zeta=1$? Can you explain why?
- B6) In the Hartree-Fock approximation, eq. (*), the 2D electron gas is fully polarized for r_s larger than ≈ 2 . Run VMC simulations of the polarized electron gas for a few values of r_s using the parameter-free “Slater-Jastrow” wave function with plane-wave orbitals and two-body correlations. Compare with the corresponding entries of Table III of Ref. [1] for the unpolarized electron gas: is the Hartree-Fock prediction accurate?