Computational Solid State Physics
First part (QMC)
Mekeup Exam, January 13th 2025

In this folder you find the following files:

- QMC_makeup_test.pdf: this file
- 2degas.pdf: Ref. [1] (in this paper, 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
- doc.pdf: documentation on the setup and qmc codes, and procedures to perform specific tasks (from the "2degas" computer lab)

You should be familiar with the use of these codes; 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.

Write your answers in a file using plain text or your favorite word processor, and keep the output files of all your simulations. At the end of the test, compress the folder with your work and send it by email to saveriomoroni@gmail.com (you may need to remove the executables).

A. Consider a free particle moving in [-1,1],

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}, \quad -1 \leq x \leq 1.$$

1) Calculate the local energy for $\Psi_1(x) = 1 - x^2$.
   Does the variance of the local energy diverge? Why?

2) Calculate the local energy and its variance for $\Psi_2(x) = \sin(\pi x)$.
   Is Ψ_2 the exact ground state wave function?

B. VMC and DMC methods

1) Is the VMC simulation a Metropolis algorithm?

2) Do the results of a VMC calculation depend on the size of the move (or time step)?

3) Does the efficiency of a VMC calculation depend on the size of the move?

4) How do we choose the size of the move in VMC?

5) Is the DMC simulation a Metropolis algorithm?

6) Do the results of a DMC calculation depend on the time step?

7) Does the efficiency of a DMC calculation depend on the time step?

8) How do we choose the time step in DMC?

C. Spin polarization transition in the 2D electron gas

1) Perform VMC simulations of $N = 21$ fully polarized electrons at $r_s = 5$, 10 and 20 with a Slater-Jastrow wave function (i.e. only two-body correlations). Comparing your variational energies with the entries E_V^{SJ} of Table III of Ref. [1] for $N = 26$, estimate the density parameter r_s^* of the spin polarization transition.

2) The estimate of r_s^* given above may be biased by finite size effects. According to Ref. [1], the size dependence of the energy for unpolarized electrons is given by eq. (19), with parameters $b_1(r_s)$ and $b_2(r_s)$ taken from Table III. Assuming that the same b_1 and b_2 are valid for polarized electrons as well, plug your variational energies $E_{N=21}$ of C.1) into eq. (19) to find the corresponding values of E_∞ (hint: for polarized noninteracting electrons, $T_\infty = 2/r_s^2$). Compare with the entries E_∞^{SJ-VMC} of Table III of Ref. [1] to update your estimate of r_s^*.

3) The value of r_s^* can be further refined by increasing the accuracy of the simulation. Choose <u>one</u> value of r_s in $\{5, 10, 20\}$, and improve the quality of the SJ variational energy of C1) by either (i) including and optimizing three-body and backflow correlations, or (ii) using the more accurate fixed-node DMC simulation, as you prefer. Compare with the corresponding improvement obtained in Ref. [1] for unpolarized electrons, using the relevant entries of Table II, and argue whether r_s^* shifts to a larger or lower value.