

Variational and Diffusion Monte Carlo simulation of the 2D electron gas: the spin-polarization transition

FILES:

- `doc.pdf`: this file
- `setup.f`: a setup fortran code
- `qmc.f`: the QMC fortran code
- `qmc.h`: a file included by `qmc.f` at compile time
- `hf.f`: a fortran code to calculate the HF energy at finite N
- `statfor.f`: fortran code for averages and statistical errors
- `statforw.f`: fortran code for weighted averages and statistical errors

INTRODUCTION:

The electron gas is a fundamental model in condensed matter physics, and one of the most successful applications of QMC. At $T = 0$, the state of the system is completely specified by the “density parameter” r_s and the spin polarization $\zeta = (N_\uparrow - N_\downarrow)/(N_\uparrow + N_\downarrow)$, where $N_{\uparrow(\downarrow)}$ is the number of spin-up(down) electrons. In 2D, $r_s = (a_0 \sqrt{\pi \rho})^{-1}$, where a_0 is the Bohr radius and ρ is the density. Note that r_s is a decreasing function of ρ , i.e. high density corresponds to small r_s and *vice versa*. Due to the soft-core, long-range nature of the Coulomb potential, the system becomes non-interacting in the limit of infinite density and crystallizes at low density (Wigner crystal), unlike normal fluids with hard-core, short-range interactions which crystallize at high density.

Using energy units of Ry and length units of $r_s a_0$, the Hamiltonian is

$$H = -\frac{1}{r_s^2} \sum_{i=1}^N \nabla_i^2 + \frac{2}{r_s} \sum_{i < j}^N \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} + \text{const}$$

where the constant is the term due to a uniform, inert background of positive charge which ensures neutrality (note that for $r_s \rightarrow 0$ both the kinetic and the potential energy diverge, but the kinetic energy diverges faster and the potential energy becomes comparatively negligible; hence the non-interacting limit at high density). The $N = N_\uparrow + N_\downarrow$ electrons are placed in a square box with periodic boundary conditions.

In the absence of interactions ($r_s \rightarrow 0$), the paramagnetic system ($N_\uparrow = N_\downarrow = N/2$) has a lower energy than the ferromagnetic system ($N_\uparrow = N, N_\downarrow = 0$), because of the larger Fermi energy of the latter. Can the interactions induce a ferromagnetic transition for larger r_s ?

In the Hartree-Fock (HF) approximation, the solution with uniform density is a Slater determinant of plane waves per spin species. The energy per particle as a function of r_s and ζ (in the limit $N \rightarrow \infty$) is analytically known:

$$E_{HF} = \frac{1}{2r_s^2} [(1+\zeta)^2 + (1-\zeta)^2] - \frac{4\sqrt{2}}{3\pi r_s} [(1+\zeta)^{3/2} + (1-\zeta)^{3/2}].$$

This function is plotted in Fig. 1 for $\zeta = 0$ (thick green) and $\zeta = 1$ (thick blue) as a function of r_s . We see that the thick blue line is lower than the thick green line for r_s larger than about 2: therefore the HF approximation predicts a polarization transition at $r_s \sim 2$.

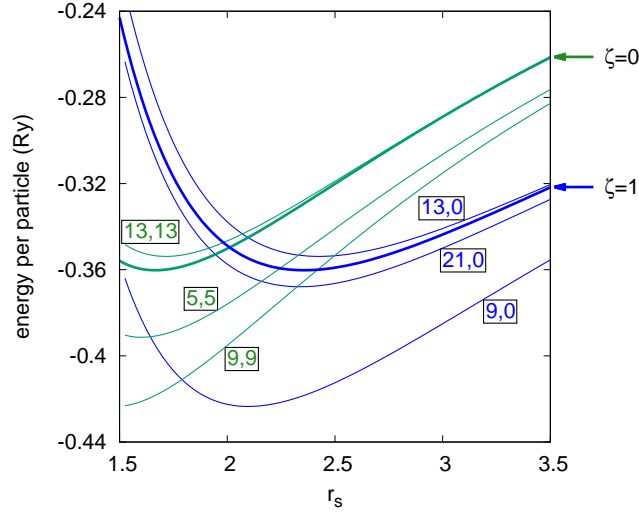


Figure 1: HF approximation: energy per particle in the thermodynamic limit (i.e. $N \rightarrow \infty$ at fixed ρ) for the paramagnetic (thick green line) and the spin-polarized (thick blue line) 2D electron gas as a function of r_s . The thin lines correspond to HF solutions with a finite number of electrons in a square box with periodic boundary conditions, each line being labeled by its respective numbers $(N_\uparrow, N_\downarrow)$.

The purpose of this test is to use a QMC code to determine whether improvements of the accuracy beyond the HF approximation shift the polarization transition to a lower or higher value of r_s .

TEST:

Follow the steps outlined below and collect your answers, as well as any comments you may want to add, in a text file (in Italian, if you prefer); keep the output files of your simulations, and include their filenames in the answers. You can organize your work in subfolders if you wish. Feel free to ask questions at any time. At the end, compress the main folder into a file and send it to saveriomoroni@gmail.com. Important note: we don't expect that you complete all of the steps. Items 1., 2. and 3. are mandatory, the other items are neither all required nor required in a particular order.

1. Compile all fortran codes (use the option `-w` to suppress warning messages and the option `-O3` to get a faster executable [here "O" is capital "o", not zero]).
2. Pick a value of r_s and a number of electrons for a polarized system (see Fig. 1; closed-shell numbers in 2D are 5, 9, 13, 25, 29, 37...), run the `setup` program and choose a Jastrow-Slater wave function (no three-body, no backflow). The two-body Jastrow function produced by the setup is a rather accurate analytic function without any variational parameter. Run a few short VMC simulations (you need to edit a `runid.in` file, where `runid` is the string you have chosen while running the setup; see keyword `vmc` in Appendix 2); after adjusting the time step to a reasonable value, run a longer VMC simulation, check for possible autocorrelations using the `statfor` code, and report the result in the answers file. This run should be long enough to see a statistically significant difference between the VMC energy and the HF energy (for the HF energy, run the `hf` code with the same values of r_s and N used in VMC).
3. Repeat the step above for a paramagnetic system, using the same value of r_s . Compare $E_{VMC}(\zeta = 0) - E_{VMC}(\zeta = 1)$ with $E_{HF}(\zeta = 0) - E_{HF}(\zeta = 1)$ and determine if the inclusion of a two-body Jastrow factor in the wave function has shifted the polarization transition towards a lower or higher value relative to HF.
4. By removing the appropriate line(s) in the `runid.sy` file (see the keywords in Appendix A), you can calculate the N -particle HF energy by Monte Carlo integration using the QMC code: do you need a VMC or a DMC simulation? Check the result you obtain against the result of the `hf` code. Of course, in the case of Monte Carlo integration you will have a statistical error. Compare the statistical error with that obtained in a simulation with the Jastrow-Slater wave function with the same number of steps. Can you explain the difference?
5. For both the paramagnetic and the polarized system chosen, calculate the DMC energy (remember to initialize a population of walkers with VMC, see the entry `istore` of the keyword `vmc`). How did you choose the time step? The DMC runs (and the VMC runs of items 2. and 3. above)

should be long enough to see a statistically significant difference between the VMC energy and the DMC energy). Does the DMC calculations further shift the polarization transition relative to VMC?

6. For one of the DMC runs of item 5., repeat the DMC simulation, first varying the time step and then varying the number of walkers; comment on the results.
7. As you can see from Fig. 1, in the HF approximation there is a strong dependence of the energy on the number of electrons, for finite systems. This is the finite-size effect. Go back to your result of item 2. pick a different number of particles and run a new VMC simulation. Compare the finite-size effect of the VMC energy and the HF energy.
8. For one of the system sizes where you already have a VMC and a DMC simulation, run the **setup** program and include three-body and backflow correlations. Optimize the wave function and run VMC and DMC simulations. For both VMC and DMC, you should find lower energies than with the previous Jastrow-Slater wave function. In particular, why is the DMC energy lower?
9. How does the improvement of the wave function affect the shift in the polarization energy? (this answer requires the optimization of the wave function for both $\zeta = 0$ and $\zeta = 1$).
10. (this has nothing to do with the polarization problem). By removing appropriate line(s) in the *runid.sy* file you can calculate the ground state energy of a system of "bosonic electrons" (in VMC, DMC or both). Why is the energy lower than for real electrons?

Appendix A: Keywords for the file *runid.sy* used in this calculation

ndim d

d (integer): dimensions of the physical space

type name number hbs2m file

define a type of particles

name (string): name of this type of particles

number (integer): number of particles of this type

hbs2m (real): value of $\hbar^2/2m$ for this type of particles

file (string): file with initial configuration(s) of the particles

v2 name_a name_b file

pair potential between particles of type **name_a** and **name_b**

name_a (string): name of a type of particles

name_b (string): name of a type of particles

file (string): name of the file with the tabulated potential

u2 name_a name_b file

two-body Jastrow factor for particles of type **name_a** and **name_b**

name_a (string): name of a type of particles

name_b (string): name of a type of particles

file (string): name of the file with the tabulated Jastrow factor

v0 value

value (real): a constant term in the potential ¹

pbx L_x [L_y [...]]

periodic boundary conditions

L_x (real): side of the simulation cell in the *x* direction

[...] (real): side of the simulation cell in the other direction(s)

kspc file

file (string): name of a file with a list of **k** points ²

¹This term comes from the splitting of the Coulomb potential into a short-range and a long-range part. See V. Natoli and D.M. Ceperley, J. Comput. Physics 117, 171 (1995).

²Needed for the orbitals in the plane-wave or backflow determinants, and/or for the **rhok** keyword

u3 name_a name_b file

three-body Jastrow factor for particles of type **name_a** and **name_b**

name_a (string): name of a type of particles

name_b (string): name of a type of particles

file (string): name of the file with the tabulated three-body function

backflow name_a name_b file

backflow correlations for particles of type **name_a** and **name_b**

name_a (string): name of a type of particles

name_b (string): name of a type of particles

file (string): name of the file with the tabulated backflow function

plane-wave name

determinant of plane waves for particles of type **name_a**

name (string): name of a type of particles

rhok name

turn on the calculation of the density fluctuation $\rho_{\mathbf{k}}$ ³

gofr

turn on the calculation of the spin-resolved pair distribution function

³ $\rho_{\mathbf{k}} = \sum_j \exp(-i\mathbf{k} \cdot \mathbf{r}_j)$, needed to calculate the long-range part of the potential and of the pair Jastrow factor in reciprocal space

Appendix B: Keywords for the file *runid.in* used in this calculation

vmc *nblocks nstep tstep istore*

define a VMC run

nblocks (integer): number of blocks

nsteps (integer): number of steps per block

tstep (real): time step (size of the move)

istore (integer): store a configuration every **istore**-th step ⁴

optimize *nconf file_1 [file_2 [...]]*

define an optimization run

nconf (integer): number of configurations for correlated sampling

file_1 (string): name of a file with a function to be optimized ⁵

[...] more files with other functions to be optimized

dmc *nblocks nstep tstep nwalkers etrial*

define a DMC run

nblocks (integer): number of blocks

nsteps (integer): number of steps per block

tstep (real): time step

nwalkers (integer): number of walkers

tstep (real): initial value of the trial energy

restart

restart a previous run; this keyword must be followed by the same **vmc** or **dmc** keyword of the previous run, with a larger **nblocks** and the same **nsteps** and **nwalkers**

⁴**istore=0** stores only the final configuration

⁵This file contains (i) number of grid points and grid step; (ii) a tabulated function with three derivatives for a spline; (iii) the name of the routine used to calculate the function; (iv) the number of variational parameters in it; (v) a list with the value of each parameter and a flag 0 or 1 which toggles the optimization of that parameter. See the files **xxx.u3**, **xxx.b**.