

Exam

1. PART A

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?

I used the following trial function

$$\psi(r_1, r_2) = e^{-\beta r_1} e^{-\beta r_2}$$

I used my own montecarlo0.jl written in julia for the MC calculation and then i analyse it using a python notebook. The output file is very big and doesn't fit in the zip because i made too many steps. In this

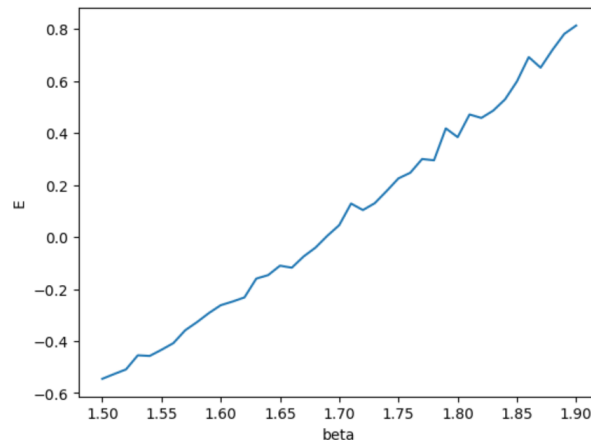


figure for the simulation we find that the optimal parameter is ~ 1.7 , it is smaller than 2 because we expect the electrons to be farther away from the nucleus in average because then they will also be further in average.

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?

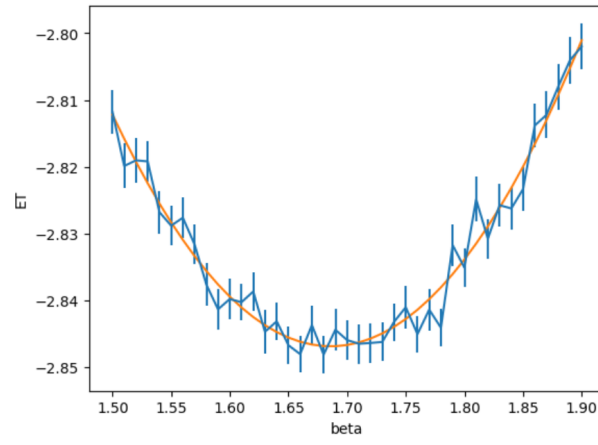
Using the same simulation as before, the jupyter notebook takes the raw output of the simulation and calculates all the statistical variables that are relevant, including the variance of the energy.

In this plot you can see the energy and its statistical error calculated by my program. If the trial function does not satisfy the cusp conditions, then the variance of the local energy will diverge, the local energy itself will not diverge because the average will still be finite, just very unstable near the cusp condition.

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).

I managed to modify the code to calculate the weights for different β , it is called montecarlo1.jl, however I did not have enough time to analyse the results.

A4 - Modify the code to calculate the Hellmann-Feynman force $F_{HF} = -\langle \partial V / \partial S \rangle$ (at least one cartesian component), where S is the position of the He atom. The exact result is F_{HF} 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.

In general I modified my code to be able to handle any number of particles, though you would have to rewrite the hamiltonian and the trial function for those. The analysis is all done in python which is very versatile.

2. PART B

B1 - I - Calculate the non-interacting energy at $r_s=1$ for a fully spin-polarized electron gas in two dimensions in the thermodynamic limit.

Without interactions (and $r_s = 1$), the hamiltonian is $-\sum_i \nabla_i^2$, whose single particle eigenstates are $\varphi_{\mathbf{k},\sigma}(\mathbf{x}) = C_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{x}}$, with eigenvalues $E_{\mathbf{k},\sigma} = |\mathbf{k}|^2$. Because electrons are fermions, the total state will be a slater determinant for the wavefunction to be antisymmetric. Because the system is completely polarized, all the electrons have the same spin σ , and because that number is fixed, and only one electron can occupy the same quantum state, that means that we will have that only one electron can have a particular momentum \mathbf{k} . This means that the energy per particle, in contrast to the unpolarized case, will be $\frac{T}{N} = \frac{1}{N} \sum_{occ} |\mathbf{k}|^2$.

Taking the thermodynamic limit, in which we take the number of particles N and the area A to infinity, while maintaining a constant density $N/A = 1/\pi r_s^2$. When taking this limit, the momentum becomes continuous and we will have that $N = \pi k_F^2 A / (2\pi)^2$ where k_F is the fermi momentum, joining these we find that $k_F = \sqrt{4/r_s^2} = 2$

And now we can change the sum of the energy per particle with the integral of k^2 and the density of states in the momentum space ($A/(2\pi)^2$), such that $\frac{T}{N} = \frac{1}{N r_s^2} \int_0^{k_F} A k^2 \frac{2\pi k dk}{(2\pi)^2} = \frac{A}{N 2\pi r_s^2} \frac{k_F^4}{4} = 2$.

If we take the formula in B5, and we associate the first term with the kinetic energy, and we have $r_s = 1$ and $\zeta = 1$ for the polarization, we also get an average energy per particle of 2.

B1 - II - Calculate the non-interacting energy at $r_s=1$ for a fully spin-polarized electron gas in two dimensions for and $N=21$ electrons in a square box with periodic boundary conditions.

Doing a VMC simulation in qmc.f for 21 up electrons (B1.tar.gz file) with $r_s = 1$ and no correlations included, after selecting a timestep of 0.05 in order to get an acceptance rate of 0.46 50%, we get the following kinetic energy statistics

EKIN	
average	1.9376716594
variance	0.0000000000
autocorrelation time	397.0100000000
n, n eff	0.5037656482

statistical error 0.0000000000

Inside the B1.tar.gz file we can find a png file with the mean local energy of each block, and we can see that we don't need to wait for thermalization. The kinetic energy for 21 polarized electrons is therefore 1.9376, which is not exactly 2 because the system is finite.

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.

I chose $r_s = 10$, and therefore I had to change the time step to 3 in order to get an acceptance rate of 0.61 50%. All the files are located in B2.tar.gz. We get the following energies

```
EKIN
average          0.0275212920
variance         0.0000002784
autocorrelation time 1.5567166703
n, n eff        128.4755304641
statistical error 0.0000465543

ELocal
average          -0.1706328843
variance         0.0000000251
autocorrelation time 1.2417320074
n, n eff        161.0653497008
statistical error 0.0000124843
```

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.

Yes, we expect to see a dependence with the time step, because DMC has an inherent error related with the time step, and ideally we the exact result is the time step 0 limit. It also depends in the number of walkers, because it introduces a bias used to control the population that only vanishes in the limit of infinite walkers.

For the timestep I took the timestep of the previous simulation and divided by 10, resulting in a timestep of 0.25. All the files are in B3.tar.gz. The energies we obtain from the simulation are.

```
ELKIN
average          0.0279737118
n,neff          101.000000    100.089372
variance         0.0000004240
autocorrelation time 1.2341034398
n eff           81.1029032622
statistical error 0.0000723079

ELocal
average          -0.1708360146
n,neff          101.000000    100.089372
variance         0.0000000265
autocorrelation time 1.1776276086
n eff           84.9923788807
statistical error 0.0000176413
```

And we can calculate the extrapolated kinetic energy as $A_{ext} = 2A_dmc - A_vmc$ for an observable A, in this case the kinetic energy, we will have 0.02842 ± 0.00009 .

B4 - Assume that eq. (19) of Ref. [1] holds for the DMC energy of the polarized electron gas with the values $b1(r_s)$ and $b2(r_s)$ 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.

$\Delta_N T$ for $N=21$ in our case is $2 - 1.93767 = 0.062328$, E_N for $N=21$ in our case is -0.17083 ± 0.00002 and therefore $E^\infty = -0.17083 - b_1(10) * 0.062328 - b_2(10)/21$, where $b_1(10) = 0.0105 \pm 0.0005$ and $b_2(10) = -0.018 \pm 0.001$. We get therefore $E^\infty = -0.17062 \pm 0.00004$.

B5 - The Hartree-Fock energy for the 2D electron gas with density parameter r_s and spin polarization in the thermodynamic limit is:

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

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?

For fully polarized ($\zeta = 1$) and $r_s = 10$, the theoretical Hartree-Fock energy is $2 * 2/2 * 10 * 2 + ((2) * (3/2)) * 4 * \text{sqr}(2)/(3 * \pi * 10) = -0.14976$. Then the correlation energy is just the difference $E_c = E^\infty - E_{HF} = -0.02085 \pm 0.00004$.

If we calculate the HF energy for an unpolarized gas we get -0.05502 , which is much lower (in absolute value, higher lower with sign into account) than what we got in the polarized system, and therefore the correlation will be greater (in absolute value, lower with sign into account). This makes sense because in an unpolarized system we can have antiparallel spins with the same momentum, and they are more tightly packed, therefore the correlations will be higher.

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?

The following are the results for three VMC simulations, stored in B6_rs.tar.gz. We will take the HF energy as the one of the infinite system, because we don't have time to extrapolate for a finite one, we expect that the shell error will be similar for all three simulations.

r_s	5
ELOCAL	
average	-0.2872009197
variance	0.0000014344
autocorrelation time	1.3114639285
n, n eff	152.5013350763
statistical error	0.0000969829
HARTREE-FOCK Energy	-0.2595305456
CORRELATION Energy	-0.0276703741
r_s	10
ELOCAL	
average	-0.1689026683
variance	0.0000001136
autocorrelation time	1.0000000000
n, n eff	200.0000000000
statistical error	0.0000238333
HARTREE-FOCK Energy	-0.1497652728
CORRELATION Energy	-0.0191373955
r_s	20
ELOCAL	
average	-0.0924123451
variance	0.0000000136

autocorrelation time	1.0000000000
n, n eff	200.0000000000
statistical error	0.0000082513
HARTREE-FOCK Energy	-0.0798826364
CORRELATION Energy	-0.0125297087

We observe that the correlation energies, compared to Table III are much lower (in absolute value). This means that correlations are much stronger in the unpolarized system than in the polarized system, which is what we expected.

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