PHYS-E0412 Computational Physics :: Homework 6

Due date 26.2.2019 at 10.00 a.m.

Variational (Quantum) Monte Carlo

This week's problem is to calculate variationally the interacting total energy of a He atom (spin singlet, $S = 0$), using Variational Monte Carlo (VMC).
The related Fortran program for interacting bosons in harmonic confinement in 2D (`HO_2D.f90`), that was discussed during the lecture on Tuesday, should be useful for solving this homework.

1. Modify the example program so that it works in 3D (this is trivial), uses the correct nuclear potential instead of the harmonic one, and has a more appropriate trial wave function of the form

$$\Psi(r_1, r_2) = \exp(-\alpha r_1) \exp(-\alpha r_2) \exp(r_{12}/(1 + \beta r_{12})) \tag{1}$$

   Hint: Now you have 2 variational parameters instead of 1. It might be easiest from the point of view of Problem 2 to put both of these in a single array.

   Calculate the variational energy and variance of the local energy using parameter values $\alpha = 2$ and $\beta = 0.5$. Report also statistical errors for both values.(3 p)

2. Modify the VMC parameter optimization routine so that it can handle more parameters than just 1. Please also try switching the Jastrow pair-correlation factor to $(1 + \beta r_{12})$. How low can you go in energy and variance, what is the Jastrow and its parameter values then? What does the variance tell you about the trial wave function? (2 p)

   A side note: In principle you can experiment freely with the trial wave function to try to optimize it further as long as you conserve the symmetry/antisymmetry properties relevant for your system. However, in the case of the Coulomb interaction there is the problem that the potential energy diverges at close distances. The wave function (and thereby the kinetic energy) can be corrected to cancel this singularity by taking into account the so-called "Kato's cusp conditions". Both of the above Jastrow forms obey these. If you see instabilities / divergencies in your experiments you are probably violating them.

3. How many hours did you spend working on this exercise?

Upload your solution in MyCourses (mycourses.aalto.fi) to the corresponding assignment. Please remember to attach your code and possible figures as well!

The Aalto-IT Linux computers have the gfortran Fortran compiler installed by default. The example program can be compiled as follows.

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gfortran -o HO_2D HO_2D.f90
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