TALENT School@MITP 2022
DMC python exercise

4/8/2022

Open the python script `DMC_exercise.py`. This script is prepared for an implementation of the DMC method to obtain the ground state energy and wave-function of the Schrödinger equation with a local interaction.

Harmonic oscillator exercise :

We first try to calculate the ground state of the 1D harmonic oscillator Hamiltonian, which in natural units $m = \hbar = 1$ reads

$$H = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2. \quad (1)$$

In the script you can find the function `dmc_step(poten,xold,eold,ntarget,dtau)` the parameters of the routine are: Note that in the code `h2m` $= \hbar^2/m$.

Table 1: DMC step subroutine

input	`xold`	old (current) walkers positions
	`eold`	old (current) energy estimate
	`poten`	the interaction, e.q V_HO or V_Morse
	`ntarget`	desired number of walkers
	`dtau`	time step
output	`xnew`	new walkers positions
	`enew`	new energy estimate

1. Complete the `step_dmc` function calculating the evolution of the walkers population via the DMC method.

2. After completion of `step_dmc` function use the python script to calculate the one dimensional HO ground state energy and wave function.

3. Introduce some smoothing procedure to extract the "best" estimate for the $E, \Delta E$.
4. Repeat the calculation changing `nwalkers` and plot the convergence of the energy as a function of `nwalkers`.
5. Repeat the calculation changing `tau` and plot the convergence of the energy as a function of τ.
6. Repeat the calculation for the Morse potential

$$V(x) = \frac{1}{2}(e^{-2x} - 2e^{-x}) \tag{2}$$

given in the code. What is the ground state energy in this case?