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H3a Diffusion Monte Carlo

Here you are asked to implement the Diffusion Monte Carlo technique. You will first study the one-dimensional harmonic oscillator problem and then the Helium atom. Atomic units (a.u.) are used, i.e. $\hbar = e = m_e = 4\pi\epsilon_0 = 1$, and the equation numbers refer to the Lecture Notes "Quantum Structure".

Task

1. Study first the one-dimensional harmonic oscillator problem. Its Hamiltonian is given by

$$\mathcal{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{k}{2}x^2$$

We use atomic units and assume that the force constant k is equal to 1 in these units, i.e.

$$\mathcal{H} = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2$$

The ground-state wavefunction is then given by

$$\psi(x) = \frac{1}{\sqrt{2\pi}}e^{-x^2/2}$$

and the ground-state energy is $E_0 = 1/2$.

The diffusion Monte Carlo method can then be implemented as

- Put N_0 walkers at random position and choose a value for E_T
- For all walkers
  - displace each walker according to the diffusive part, Eq. (61)
  - evaluate the weight factor $W(x)$ and eliminate or create walkers according to Eq. (62)
- Update E_T according to Eq. (63) so that the number of walkers will stabilize around the value N_0
- Repeat many times

For this problem a suitable number of walkers N_0 is a few hundred. The time step $\Delta\tau$ should be less than 1. You could test a few values in the range $0.01 < \Delta\tau < 0.1$. Plot your result for E_T as function of time τ. It is also useful to plot the number of walkers as function of time τ. Does the simulation result stabilize, equilibrate, when τ is increasing? It should approach the correct ground-state energy. When the system has stabilized you can use that part of the simulation to determine the ground-state energy. It is instructive to also plot the density $n(x) = |\psi(x)|^2$ as function of x. Normalize and compare with the exact result for the ground-state density. To get better statistics for the density make an average over time. (6p)

2. Consider nowthe Helium atom.

$$\mathcal{H} = -\frac{1}{2}(\nabla_1^2 + \nabla_2^2) - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}}$$

Use the same algorithm as above. However in this case the walkers are not moving in one-dimension. You have to generalize to 6 dimensions. In this case you will find that the algorithm is less efficient. It takes a very long time to reach an accurate sampling due to the divergence of the potential. However, try to convince yourself that the program is working correctly in 6 dimensions. (0p)

3. The problem associated with the divergent potential can be solved using importance sampling. One then introduces a trial wavefunction $\Psi_{\mathsf{T}}(\mathcal{R})$ that mimics the real wave function $\Psi(\mathcal{R})$. Here, $\mathcal{R}$ denote the position in 6 dimensions of the two electrons. You should use the same trial wave-function has in the homework problem H2b Variational Monte Carlo. The original Schrödinger equation is then transformed to a Fokker-Planck equation (see Sec. 6.3 in the Lecture Notes "Quantum structure") for the function $f(\mathcal{R}, \tau) = \Psi_{\mathsf{T}}(\mathcal{R})\Psi(\mathcal{R}, \tau)$. The pure diffusive step in Eq. (61) is replaced by a guided step, as in Eq. (44). The walkers are pushed into important regions. The technique, guided sampling, is described in Sec. 5.3 in the Lecture Notes "Quantum structure".

   Perform a Diffusion Monte Carlo study of Helium. In this case do not try to extract the density $n(\mathcal{R})$ from $f(\mathcal{R})$. Also do not try to correct for the time-step error (described in Sec. 5.3 in the Lecture Notes "Quantum structure") introduced by the finite value of $\Delta\tau$. What value do you obtain for the ground-state energy of Helium? (8p)

4. Implement now the correction for the time-step error. Perform long simulations and estimate also the error for the ground-state energy. Compare result from the simulation without and with correction for the time-step error. Does the correction improve on the value for the ground-state energy? Give your final result for the ground-state energy with error bars. (2p)