

Exercise Lecture X

Variational Monte Carlo (VMC) - II part 3D examples

1. Hydrogen atom.

- (a) We want to find numerically the ground state of the H atom. We want to find numerically the ground state. The hamiltonian is: $\mathcal{H} = p^2/(2m) - e^2/r$; It is convenient to use atomic units ($\hbar = 1$, $m_e = 1/2$, $e^2=2$, and therefore to measure all length in terms of Bohr radius, $a_0 = \hbar^2/(me^2)$, the energies in Rydberg, $Ry = me^4/(2\hbar^2)$). Consider the trial wavefunction $\psi(\mathbf{r}) = \psi(r) = e^{-r/a}$, where a is a variational parameter. calculate the optimal value of a and the corresponding energy.

Hints:

1) you may reduce the problem (spherical part) to a 1D problem. Pay attention that

$$\langle E_L \rangle = \frac{\int \psi^2(r) E_L(r) d\mathbf{r}}{\int \psi^2(r) d\mathbf{r}} = \frac{\int \psi^2(r) E_L(r) 4\pi r^2 dr}{\int \psi^2(r) 4\pi r^2 dr}$$

and therefore the sampling probability is $r^2\psi^2(r)$ and not just $\psi^2(r)$.

2) Pay attention close to the origin!

- (b) Approach the problem keeping a 3D formulation, considering the isotropy of the trial move (The displacement is a vector!)