Variational Monte Carlo: Practical Session

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(adapted from previous school's presentation by B. Busemeyer)

Classes in python:

Class Hamiltonian

Member data:	Member functions:
Self.Z (ion charge)	Def compute_energy(self, pos) (compute an energy)

How to use:

1. Create instance: calls __init__(self,…)
   ham=Hamiltonian(Z=2)
2. Use functions
   ham.compute_energy(pos1)
   ham.compute_energy(pos2)

Goals

For a He atom:

1. Implement pieces (evaluation and sample)
2. Explore parameters
3. Explore the effect of including correlation in the wavefunction

Details are provided in “instructions.pdf”

Nota bene:

- Test early and often
- Do simplest implementation first
- Avoid solutions until you've been stuck for quite some time. Ask questions first!!!

Discuss interpretation question with group

What are we trying to do in VMC

- Compute an expectation value for a known (parameterized) wavefunction

$$\langle E \rangle = \int d^{3N} \Psi^*(R,P) \hat{H} \Psi(R,P)$$

R: positions
P: parameters

$$= \int d^{3N} |\Psi(R,P)|^2 \frac{\hat{H}\Psi(R,P)}{\Psi(R,P)}$$

Probability distribution

Some function of R:
E(R) "local energy"

In this code

1. Including all pieces necessary to evaluate a gaussian wavefunction (eventually times a Jastrow factor) for the local energy
2. Using the metropolis algorithm to be able to sample the probability distribution from the square of the wavefunction
3. Once we can evaluate these for generic choices of parameter, can think about optimization