Computational Quantum Physics
Exercise 5

FS 10
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Problem 5.1 Variational Monte Carlo - Harmonic Oscillator

Consider a single particle confined in a one dimensional harmonic oscillator, ie.

$$\hat{H} = -\frac{1}{2}\partial_x^2 + \frac{1}{2}x^2 \tag{1}$$

Now, employ a trial wavefunction $\phi_c(x) = \exp(-cx^2)$, with c as the variational parameter to investigate this problem. The corresponding energy functional can be written as

$$E[c] = \frac{\int dx \phi_c^*(x)\hat{H}\phi_c(x)}{\int dx \phi_c^*(x)\phi_c(x)}. \tag{2}$$

We would like to perform this integral with importance sampling by assigning to configurations x the weight

$$W(x) = \frac{\phi_c^*(x)\phi_c(x)}{\int dx \phi_c^*(x)\phi_c(x)}. \tag{3}$$

We therefore perform a random walk with the Metropolis algorithm, where the acceptance probability is given by

$$P(x_i \to x_f) = \min\left\{1, \frac{\phi_c^*(x_f)\phi_c(x_f)}{\phi_c^*(x_i)\phi_c(x_i)}\right\}. \tag{4}$$

To evaluate the energy functional, calculate the expectation value and the standard error of

$$\epsilon[c] = \frac{\hat{H}\phi_c(x)}{\phi_c(x)} \tag{5}$$

- Evaluate E[c] via VMC using the above ansatz for c = 0.3, 0.4, 0.5, 0.6, 0.7. Plot E[c] vs c. Please include errorbar and observe that the variance at c=0.5 is exactly zero. (This is known as zero variance principle.)
- What will you do if you want to estimate first excited state energy of the same problem using VMC?

Note: In the random walk, propose a new value of x within an unit radius from the old value of x.