

# Computational Quantum Physics Exercise 6

## Problem 6.1 Variational Monte Carlo - Harmonic Oscillator

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

$$\hat{H} = -\frac{1}{2}\partial_x^2 + \frac{1}{2}x^2 \quad (1)$$

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

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

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

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

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

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

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

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

- 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 errorbars 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  $x$ .