**Computational Physics II 5640 Spring 2018**

**Project Assignment 5**

Due: Friday May 11

**1. Variational Quantum Monte Carlo**. Consider Schrodinger equation for 1D harmonic oscillator:

$$-\frac{1}{2}\frac{d^2\psi(x)}{dx^2} + \frac{x^2}{2}\psi(x) = E\psi(x). \tag{1}$$

Here we employ Monte Carlo method to study the variational wave function. We consider the trial wave function $\psi_\alpha(x) \propto \exp(-\alpha x^2)$. Show that the local energy is given by

$$E_L(x) = \alpha + x^2(\frac{1}{2} - 2\alpha^2). \tag{2}$$

Write a Markov-chain Monte Carlo code (essentially the 1D random walk) to compute the expectation $\langle E_L\rangle$ and the variance $\langle E_L^2\rangle - \langle E_L\rangle^2$ of the local energy, and plot them as functions of the variational parameter $\alpha$; see Fig. 1. The minimum of both quantities occur at $\alpha = 0.5$ corresponding to the exact ground-state solution.

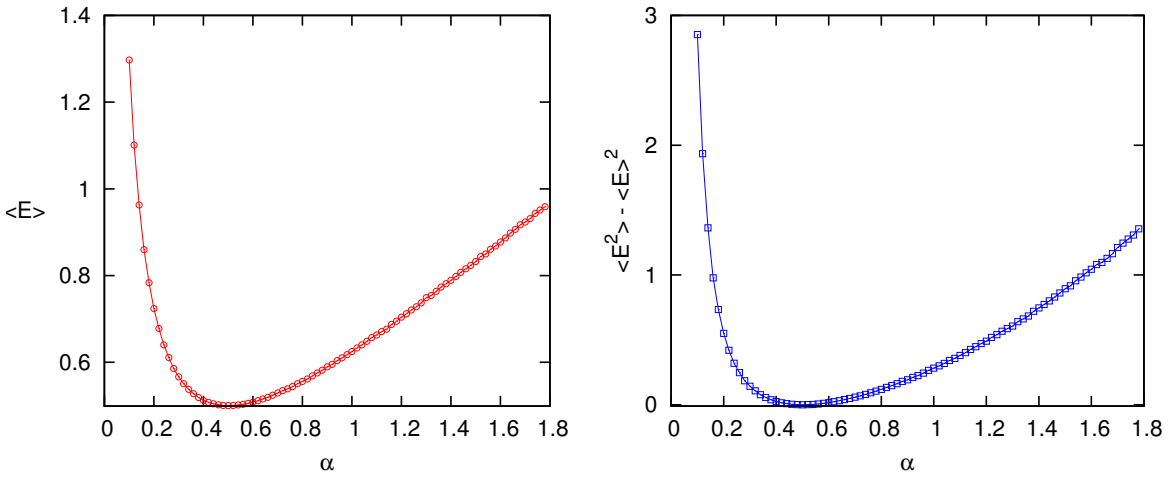


Figure 1: The expectation value and variance of the local energy $E_L(x)$ computed using random-walk Metropolis method for the 1D harmonic oscillator problem.

Next show that the gradient of expectation value of $E_L$ is given by formula:

$$\frac{d\langle E_L\rangle}{d\alpha} = 2\left(\left\langle E_L \frac{d\ln\psi}{d\alpha}\right\rangle - E_L\left\langle \frac{d\ln\psi}{d\alpha}\right\rangle\right). \tag{3}$$

Here $\langle\cdots\rangle$ means Monte Carlo averages which are computed using the random-walk code. Starting from some arbitrary value for $\alpha$, use the damped steepest descent method to update $\alpha$:

$$\alpha^{(n+1)} = \alpha^{(n)} - \gamma\,\frac{d\langle E_L\rangle}{d\alpha}. \tag{4}$$

The optimum $\alpha$ which minimizes the local energy can be reached in a few steps, as demonstrated in Fig. 2.

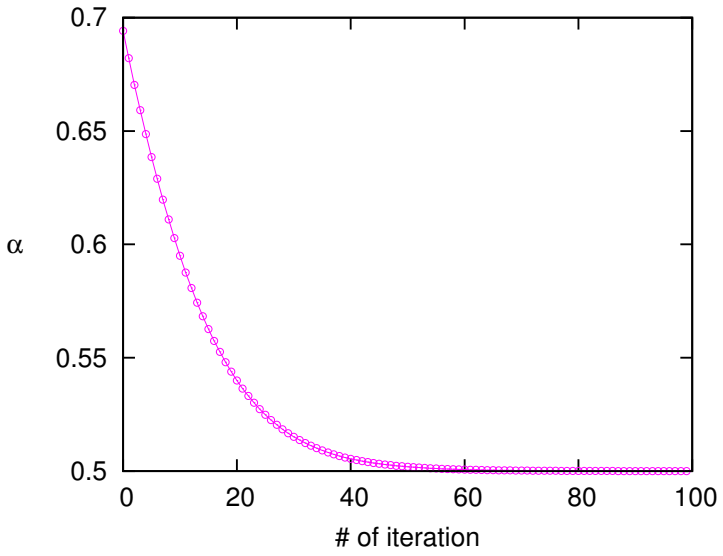


Figure 2: The variational parameter $\alpha$ versus number of iteration in a gradient descent minimization. Initial $\alpha = 0.7$ and $\gamma = 0.05$.

**2. Diffusion Quantum Monte Carlo**. Implement the diffusion Monte Carlo (DMC) method to study the single-particle Schrodinger equation in three dimensions:

$$i\frac{\partial \Phi}{\partial t} = -\frac{1}{2}\nabla^2\Phi + V(\mathbf{r})\,\Phi \tag{5}$$

Here we have used units such that $\hbar = 1$, $m = 1$. The "imaginary time" Schrodinger equation describes a diffusion-death-birth process of particles. The corresponding Green's function has the form:

$$G(\mathbf{r}', \mathbf{r}; \Delta\tau) = e^{\Delta\tau(E_T - V(\mathbf{r}'))}\frac{1}{\sqrt{2\pi\Delta\tau}}\,e^{-\frac{|\mathbf{r}'-\mathbf{r}|^2}{2\Delta\tau}} = W(\mathbf{r}')\,G_{\rm diff}(\mathbf{r}', \mathbf{r}; \Delta\tau). \tag{6}$$

The DMC algorithm is based on the above Green's function. Specifically, we prepare initially $M_0$ random walkers. Then repeat the following steps:

**begin**

**for** $\forall$ walkers **do**

(1) update its position $\mathbf{r}_{\rm new} = \mathbf{r}_{\rm now} + \sqrt{\Delta\tau}\,(\xi_1, \xi_2, \xi_3)$,
where $\xi_i$ are Gaussian random variables with zero mean and unit variance.

(2) evaluate $W := \exp[\Delta\tau(E_T - V(\mathbf{r}_{\rm new}))]$.
let $s := [W]$, where $[W]$ is the integer part of $W$.
generate a random number $r$ uniformly distributed in $[0, 1]$.
**if** $r < (W - [W])$ **then** $s := s + 1$.

(3) **if** $s = 0$ **then** remove this walker.
**else** create $s - 1$ copies of this walker (total number of same walker at $\mathbf{r}_{\rm new}$ is $s$).

**end for**

update reference energy $E_T := E_T + \alpha\,\ln(M_T/M)$,
$M$ is the current number of walkers, and $M_T$ is the target number, $\alpha$ is a small number.

**end**

In this homework, apply the DMC algorithm to study a 3D harmonic oscillator with the potential $V(\mathbf{r}) = \frac{|\mathbf{r}|^2}{2}$ (the spring constant $k = 1$), which has a ground state energy and wavefunction:

$$E_0 = \frac{3}{2}, \qquad\qquad \Phi_0(\mathbf{r}) = \frac{e^{-|\mathbf{r}|^2/2}}{(2\pi)^{3/2}}, \tag{7}$$

The ensemble of the walkers provide a sampling of the wavefunction $\Phi(\mathbf{r})$ itself (not the squared one). Plot the histogram of $4\pi r^2\Phi(r)$ from DMC and compare with exact solution; see Fig. 1. Also plot the distribution of reference energy $E_T$ and number of walkers $M$ using the histogram method. The average $\langle E_T\rangle$ should give the ground state energy $E_0 = 3/2$.

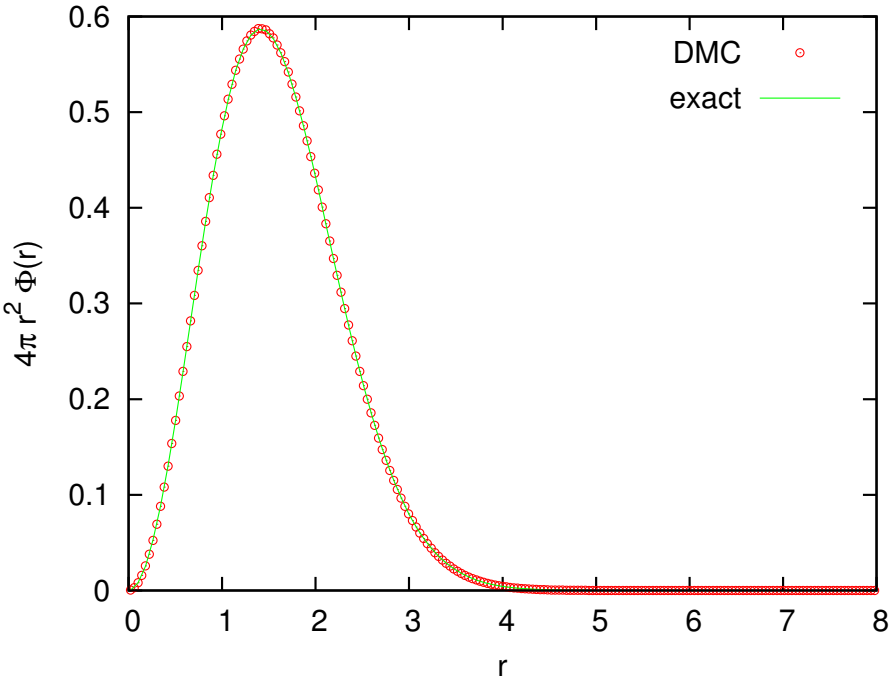


Figure 3: Ground-state wavefunction obtained from DMC simulation compared with exact solution $4\pi r^2\,\Phi_0(r)$. Numerically, this is given by the histogram of $|\mathbf{r}_i| = \sqrt{x_i^2 + y_i^2 + z_i^2}$, where $\mathbf{r}_i$ is the position vector of the random walkers in DMC.