# Quantum Monte Carlo Simulation

We use random walks to obtain the ground state (i.e., the eigenstate with the lowest energy) of a quantum system [1]. To understand this method, we substitute $\tau = it$ into the time-dependent Schrödinger equation (in one dimension) to obtain

$$\frac{\partial}{\partial \tau}\psi(x,\tau) = -\frac{H}{\hbar}\psi(x,\tau) = \frac{\hbar}{2m}\frac{\partial^2}{\partial x^2}\psi(x,\tau) - \frac{V(x)}{\hbar}\psi(x,\tau). \tag{1}$$

If we retain only the first term in the right-hand side, this is the diffusion equation we have studied in the lecture on "Monte Carlo Simulation on Stochastic Processes". We can thus interpret the wave function $\psi(x,\tau)$ as a probability density with a diffusion constant $D = \hbar/2m$. We have learned that random walks can be used to find the solution to the diffusion equation. The second term, on the other hand, is a growth term, i.e., the population density of the random walkers at $x$ grows or decays for a negative or positive potential $V(x)$ value, respectively.

The general solution to Eq. (1) is written in terms of the eigenstates, $\phi_n(x)$, and eigenenergies, $E_n$, of the Hamiltonian $H$. (We sort the eigenenergies, $E_n$, in the ascending order, with $E_0$ being the ground state energy.)

$$\psi(x,\tau) = \exp(-H\tau/\hbar)\psi(x,0) = \sum_n c_n \phi_n(x)\exp(-E_n\tau/\hbar), \tag{2}$$

where the weight of the initial wave function projected onto the $n$-th eigenstate is

$$c_n = \int dx \phi_n(x)\psi(x,0). \tag{3}$$

Consider the long-time limit of Eq. (2). Noting that the ground state decays slowest among all the eigenstates, we obtain

$$\lim_{\tau\to\infty}\psi(x,\tau) = c_0\phi_0(x)\exp(-E_0\tau/\hbar). \tag{4}$$

Thus the histogram of random walkers will be proportional to the ground-state wave function, $\phi_0(x)$, in the long-time limit.

The only problem of the above procedure is that the population of walkers will decay to zero if $E_0 > 0$ or explode to infinity if $E_0 < 0$. To avoid this problem, we will measure the energy from a reference energy, $V_{\text{ref}}$, which is adjusted to achieve a stationary population of random walkers. As shown in Appendix, $E_0$ can be determined from the relation,

$$E_0 = \langle V \rangle = \frac{\int_{-\infty}^{\infty} V(x)\psi(x,\tau)dx}{\int_{-\infty}^{\infty}\psi(x,\tau)dx}, \tag{5}$$

or it can be estimated by finite sampling,

$$E_0 = \langle V \rangle = \frac{1}{N}\sum_{i=1}^{N} V(x_i), \tag{6}$$

where $N$ is the number of random walkers and $x_i$ is the position of the $i$-th walker.

Quantum Monte Carlo simulation discretizes imaginary time in unit of $\Delta\tau$. During one time step,

$\Delta\tau$, each random walker moves either to the right or left by step length, $\Delta s$, which is related to $\Delta\tau$ by $(\Delta s)^2 = 2D\Delta\tau$. (Note that we have proven this relation in the lecture on "Monte Carlo Simulation of Stochastic Processes, when we derive the diffusion equation from random walks. The diffusion constant $D = 1/2$ in the atomic unit, $\hbar = m = 1$.) The reference potential can be estimated from the mean potential $\langle V \rangle$ and the change in the number of random walkers during $\Delta\tau$ as follows.

$$V_{\text{ref}} = \langle V \rangle - \frac{N(\tau + \Delta\tau) - N(\tau)}{N(\tau)\Delta\tau}, \tag{7}$$

as shown in Appendix.

This leads to a simple quantum Monte Carlo simulation algorithm shown below.

(Quantum Monte Carlo Algorithm)

1. Place $N_0$ walkers at the initial set of positions $x_i$.
2. Compute the reference energy, $V_{\text{ref}} = \Sigma_i V(x_i)/N_0$.
3. For each walker,
   a. Randomly move the walker to the right or left by a fixed step length $\Delta s$.
   b. Compute $\Delta V = V(x) - V_{\text{ref}}$ and a random number $r$ in the range [0, 1]. If $\Delta V > 0$ and $r < \Delta V \Delta\tau$, then remove the walker. If $\Delta V < 0$ and $r < -\Delta V \Delta\tau$, then add another walker at $x$. Otherwise, just leave the walker at $x$.
4. Compute the mean potential energy (6) and the actual number of random walkers. The new reference potential is given by Eq. (7). The average $\langle V \rangle$ is an estimate of the ground state energy.
5. Repeat steps 3–4 until the estimates of the ground state energy $\langle V \rangle$ have reached a steady state value with only random fluctuations. Average $\langle V \rangle$ over many Monte Carlo steps to compute the ground state energy.

The program, qmwalk.c, implements this algorithm for a harmonic potential, $V(x) = x^2/2$, in the atomic unit. Initially, the walkers are randomly distributed within a distance $w_0$ of the origin. Input parameters are the desired number of walkers $N_0$, the number of Monte Carlo steps per walker *mcs*, and the step length *ds*. The program computes the current number of walkers $N$, the current estimate of the ground state energy, and the value of $V_{\text{ref}}$. Initial part of the samples is discarded in the averages to approximate equilibration.

The following figure shows the time average of the mean potential $\langle V \rangle$ (calculated at the *imcs*-th Monte Carlo step as the accumulated sum of $\langle V \rangle$ over *imcs* steps, *Esum*, divided by *imcs*) and the estimate of $V_{\text{ref}}$ for $N_0 = 50$, $ds = 0.1$, and $mcs = 500$.

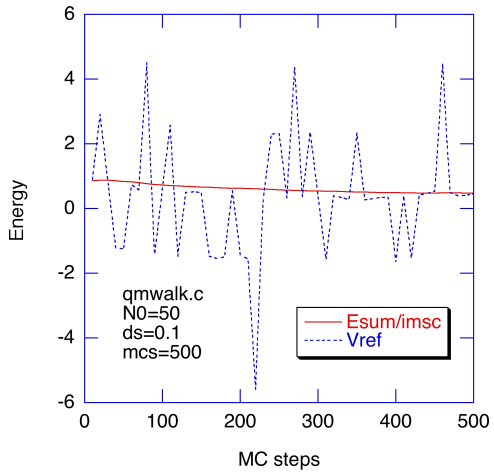


**Figure**: Time average of the mean potential $\langle V \rangle$ (denoted as *Esum*/*imcs*) and the estimate of $V_{\text{ref}}$ as a function of quantum Monte Carlo steps, *imsc*.

The following figure shows the histogram of the random walkers from the same simulation.

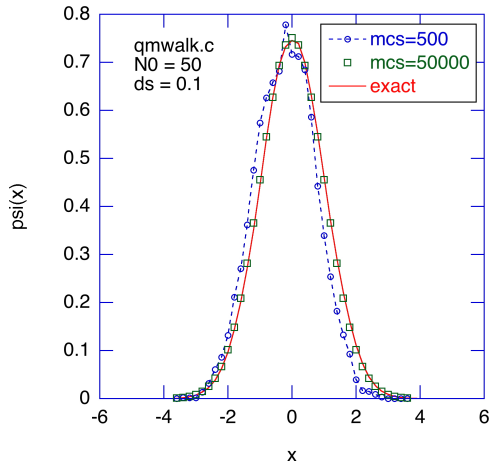


**Figure**: Histograms of random walkers in quantum Monte Carlo simulations for *mcs* = 500 and 50,000, compared with the exact solution, $\psi_0(x) = \pi^{-1/4} \exp(-x^2/2)$.

## Appendix: Derivation of Equations (5) and (7)

Let us rewrite the imaginary-time Schrödinger equation (1), including the reference potential.

$$\frac{\partial}{\partial \tau}\psi(x,\tau) = \frac{\hbar}{2m}\frac{\partial^2}{\partial x^2}\psi(x,\tau) - \frac{V(x)-V_{\text{ref}}}{\hbar}\psi(x,\tau) \tag{A1}$$

By integrate this equation with respect to $x$, we obtain

$$\begin{aligned}\int_{-\infty}^{\infty}\frac{\partial}{\partial \tau}\psi(x,\tau)\,dx &= \left[\frac{\hbar}{2m}\frac{\partial}{\partial x}\psi(x,\tau)\right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\frac{V(x)}{\hbar}\psi(x,\tau)\,dx + \frac{V_{\text{ref}}}{\hbar}\int_{-\infty}^{\infty}\psi(x,\tau)\,dx \\ &= -\int_{-\infty}^{\infty}\frac{V(x)}{\hbar}\psi(x,\tau)\,dx + \frac{V_{\text{ref}}}{\hbar}\int_{-\infty}^{\infty}\psi(x,\tau)\,dx\end{aligned} \tag{A2}$$

The kinetic-energy term vanishes, because the wave function and hence its derivative are 0 at $x \to \pm\infty$.

Now note that, in the long-time limit, the wave function is

$$\psi(x,\tau) \approx c_0 \phi_0(x) \exp\left(-(E_0 - V_{\text{ref}})\tau / \hbar\right). \tag{A3}$$

By differentiating Eq. (A3) with respect to time, we obtain

$$\frac{\partial}{\partial \tau}\psi(x,\tau) \approx \frac{V_{\text{ref}} - E_0}{\hbar}\psi(x,\tau). \tag{A4}$$

Substituting Eq. (A4) into (A2), we obtain

$$\int_{-\infty}^{\infty} \frac{V_{\text{ref}} - E_0}{\hbar}\psi(x,\tau)dx = -\int_{-\infty}^{\infty} \frac{V(x)}{\hbar}\psi(x,\tau)dx + \frac{V_{\text{ref}}}{\hbar}\int_{-\infty}^{\infty}\psi(x,\tau)dx. \tag{A5}$$

The terms proportional to $V_{\text{ref}}$ cancel, and we finally obtain

$$\frac{E_0}{\hbar}\int_{-\infty}^{\infty}\psi(x,\tau)dx = \int_{-\infty}^{\infty}\frac{V(x)}{\hbar}\psi(x,\tau)dx, \tag{A6}$$

which is equivalent to Eq. (5).

To derive Eq. (7), note that the number of random walkers $N(\tau)$ is written as

$$N(\tau) = \int_{-\infty}^{\infty}\psi(x,\tau)dx. \tag{A7}$$

Equation (A2) can then be written as

$$\frac{d}{d\tau}N = \frac{V_{\text{ref}} - \langle V \rangle}{\hbar}N(\tau). \tag{A8}$$

Suppose we have estimated the current rate of change in $N$. We will then set $V_{\text{ref}}$ in order to counter-balance this change so that a steady population is, i.e.,

$$-\frac{d}{d\tau}N\bigg|_{\text{current}} = \frac{V_{\text{ref}}^{\text{new}} - \langle V \rangle}{\hbar}N(\tau), \tag{A9}$$

or

$$\frac{V_{\text{ref}}^{\text{new}}}{\hbar} = \frac{\langle V \rangle}{\hbar} - \frac{dN/d\tau}{N(\tau)}. \tag{A10}$$

The time-discretized form of Eq. (A.10) gives Eq. (7).

## References


1. H. Gould and J. Tobochnik, *An Introduction to Computer Simulation Methods, Second Edition* (Addison-Wesley, 1995).