Note on Quantum Monte Carlo (QMC) Programming

QMC Recap: Solving Imaginary-Time Schrödinger Equation by Random Walk

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x,t)$$

$$\downarrow\ \tau \equiv it$$

$$i\hbar\frac{\partial}{-i\partial\tau}\psi = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi$$

$$\therefore\ \frac{\partial}{\partial\tau}\psi = \left[\frac{\hbar}{2m}\frac{\partial^2}{\partial x^2} - \frac{V(x)}{\hbar}\right]\psi$$

By introducing population control, V_{ref},

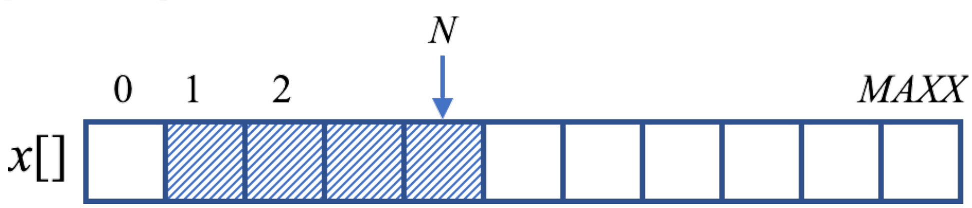
$$\underbrace{\frac{\partial}{\partial\tau}\psi}_{\text{population−change rate}} = \left[\underbrace{\underbrace{\frac{\hbar}{2m}}_{D=\frac{1}{2}\,[\text{a.u.}]=\frac{(ds)^2}{2dt}}\frac{\partial^2}{\partial x^2}}_{\text{diffusion}} + \underbrace{\frac{V_{\text{ref}} - V(x)}{\hbar}}_{\text{birth/death rate}}\right]\psi$$

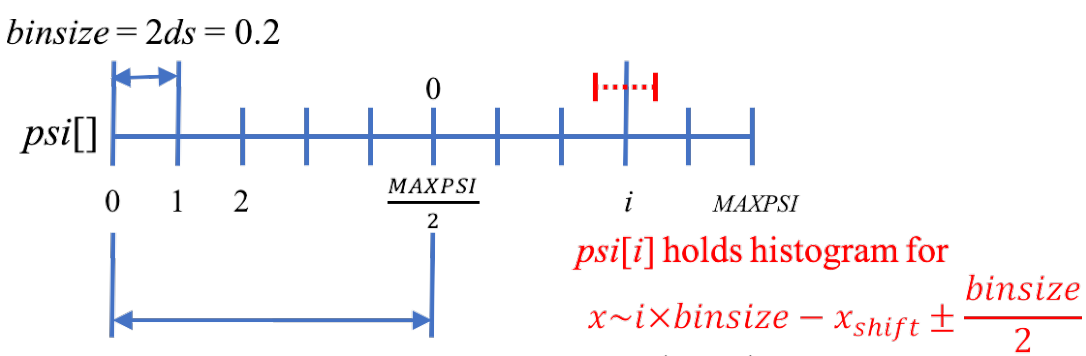
Data Structures

int N // Number of random walkers

double $x[MAXX+1]$ // $x[i]$ ($i = 1,\ldots,N$) is the position of the i-th random walker ($MAXX = 2000$)

double $psi[MAXPSI+1]$ // Histogram of random walkers ($MAXPSI = 1000$)





$$x_{shift} = binsize(0.2)\times\frac{MAXPSI(=1000)}{2} = 100.0$$

Algorithm

$N \leftarrow N_0 = 50$ // Initialize the number of random walkers to the desired value

$x[1{:}N] \leftarrow$ uniform random number in the range [-1,1] // 2*rand*()/(double)*RAND_MAX*-1

$V_{\text{ref}} \leftarrow \frac{1}{N}\sum_{i=1}^{N} V(x[i])$ // Initial reference energy, where $V(x) = \frac{x^2}{2}$ is the harmonic potential

Reset the histogram, $psi[0{:}MAXPSI] \leftarrow 0$

for *step* = 1 to $nequil = 0.4 \times mcs = 0.4 \times 500 = 200$ // Equilibrate random walkers
    walk()

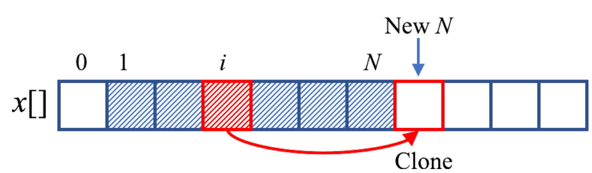
for *step* = 1 to $mcs = 500$ // Main MC loop for sampling
    walk()
    Add the *N* random walkers' positions to the histogram, *psi*[]

Function *walk*(): Random Walk with Birth/Death

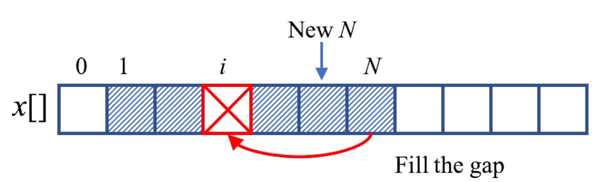
$N_{\text{in}} \leftarrow N$ // Number of walkers at the beginning of this MC step

$V_{\text{sum}} \leftarrow 0.0$ // Reset the accumulator to sum the potential energies of walkers

for (i=N_{in}; i>=1; --i) // In descending order to handle birth/death
    // Random walk by step ds = 0.1
    if (rand()%2 == 0)
        $x[i]$ += ds
    else
        $x[i]$ -= ds



    // Birth or death of walkers
    $potential \leftarrow V(x[i]) = x^2/2$
    $dV \leftarrow potential - V_{\text{ref}}$
    if (dV < 0) // Check whether to duplicate the walker
        if (*rand*()/(double)*RAND_MAX* $< -dV \times dt$) // Duplicate the walker with probability $-dV \times dt$
            ++N
            $x[N] = x[i]$ // Clone a new walker at the same position
            V_{sum} += 2×$potential$ // Factor 2 since two walkers at the same position
        else
            V_{sum} += $potential$ // Only one walker
    else // Check whether to remove the walker
        if (*rand*()/(double)*RAND_MAX* $< dV \times dt$) // Remove the walker with probability $dV \times dt$
            $x[i] \leftarrow x[N]$ // Fill the gap created by death
            --N
        else
            V_{sum} += $potential$ // The walker survived



$V_{\text{average}} \leftarrow V_{\text{sum}}/N$

$V_{\text{ref}} \leftarrow V_{\text{average}} - \frac{N-N_0}{N_0 \times dt}$ // New reference energy; note $dt = ds^2 = 0.01$