# Quantum Monte Carlo

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## Introduction

Here I will describe various Monte Carlo methods used in solving quantum many body systems. I will start by describing Variational Monte Carlo (VMC) which is the most basic, and then I will describe Diffusion Monte Carlo (DMC). DMC is difficult to do when spin and isospin are included so I will then describe a method used to make the spin and isospin sampling easier called Auxiliary Field Diffusion Monte Carlo (AFDMC).

## Variational Monte Carlo

There are many good books that describe the basics of the VMC method, but I found the explanation in [1] to be particularly useful, and I have drawn heavily from this paper to build my understanding of VMC and DMC.

### Monte Carlo Integration

Before explaining variational Monte Carlo (VMC) I am going to describe the method for performing Monte Carlo integration. Assume that we are trying to integrate the function

$$I = \int g(\mathbf{R}) d\mathbf{R}. \tag{1}$$

This can be rewritten as

$$I = \int f(\mathbf{R}) P(\mathbf{R}) d\mathbf{R} \tag{2}$$

where $f(\mathbf{R}) = g(\mathbf{R})/P(\mathbf{R})$, and $P(\mathbf{R})$ is the importance function (probability density). In our case $P(\mathbf{R})$ can be interpreted as $\langle\psi_T|\psi_T\rangle$ where $|\psi_T\rangle$ is the trial wave function. Also note that $\mathbf{R} = (\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_n)$, where $\mathbf{r}_i$ is the position of the ith particle, and a specific $\mathbf{R}$ is called a *walker*. Now you say that the integral looks like the expectation value of the random variable $f(\mathbf{R})$ (Think of $\left\langle \hat{H} \right\rangle = \int_{-\infty}^{\infty} \langle\psi| \hat{H} |\psi\rangle$).

Now the integral can be determined by drawing an infinite number of samples from $f(\mathbf{R})$ and computing the average.

$$I = \lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} f(\mathbf{R}_n) \tag{3}$$

The integral can then be approximated by

$$I \approx \frac{1}{N}\sum_{n=1}^{N} f(\mathbf{R}_n). \tag{4}$$

Notice that by the central limit theorem if $f(\mathbf{R})$ has mean $\mu$ and standard deviation $\sigma^2$ then $I$ will have mean $\mu$ and standard deviation $\sigma/\sqrt{N}$.

**The Metropolis Algorithm**

Often times sampling from the distribution $P(\mathbf{R})$ is difficult because $P(\mathbf{R})$ is complicated and difficult to invert. The metropolis algorithm allows us to sample complicated $P(\mathbf{R})$'s. The steps are as follows.

1. Start at some random walker $\mathbf{R}$.
2. Propose a move to a new position $\mathbf{R}'$, pulled for a distribution $T(\mathbf{R} \leftarrow \mathbf{R}')$.
3. The probability of accepting the move is given by

$$A(\mathbf{R}' \leftarrow \mathbf{R}) = \min\left(1, \frac{T(\mathbf{R}' \leftarrow \mathbf{R})P(\mathbf{R}'))}{T(\mathbf{R}' \leftarrow \mathbf{R})P(\mathbf{R}))}\right). \tag{5}$$

   $T(\mathbf{R}' \leftarrow \mathbf{R})$ can be 1 or a Gaussian centered around the current walker, or something else entirely. A random number is then pulled from $r = U(0,1)$, and the move is accepted if $r < A(\mathbf{R}' \leftarrow \mathbf{R})$.

4. Repeat from step 2.

**VMC**

To do VMC you first start with a trail wave function $\Psi_T$. The accuracy of VMC is sensitive to the choice of $\Psi_T$. The trial wave function is then used to find a rigid upper bound on the ground state energy, $E_0$.

$$E_V = \frac{\int \Psi_T^*(\mathbf{R})\hat{H}\Psi_T(\mathbf{R})d\mathbf{R}}{\int \Psi_T^*(\mathbf{R})\Psi_T(\mathbf{R})d\mathbf{R}} \leq E_0 \tag{6}$$

The methods above are used to evaluate this integral which can be written as

$$E_V = \frac{\int |\Psi_T(\mathbf{R})|^2[\Psi_T^{-1}(\mathbf{R})\hat{H}\Psi_T(\mathbf{R})d\mathbf{R}]}{\int |\Psi_T(\mathbf{R})|^2 d\mathbf{R}}. \tag{7}$$

Random walkers are generated, $\{\mathbf{R}_n : n = 1, N\}$, from the distribution $P(\mathbf{R}) = |\Psi_T(\mathbf{R})|^2/\int |\Psi_T(\mathbf{R})|^2 d\mathbf{R}$. The local energy at each point is found using $E_L(\mathbf{R}) = \Psi_T^{-1}(\mathbf{R})\hat{H}\Psi_T(\mathbf{R})$. Now rewriting $E_V$ in terms of $E_L$ we get

$$E_V = \int P(\mathbf{R})E_L(\mathbf{R})d\mathbf{R}. \tag{8}$$

The local energy can then be sampled using the Metropolis method described above to give the energy.

$$E_V \approx \frac{1}{N}\sum_{n=1}^{N} E_L(\mathbf{R}_n). \tag{9}$$

At this point certain parameters in $\Psi_T$ can be varied until a minimum in the energy if found. A minimum in the energy will be produced when $\Psi_T \to \Psi_0$.

# Diffusion Monte Carlo

This explanation also draws heavily from [1], but also draws a good deal from [2]. The time dependent Schrödinger equation is

$$\hat{H}\Psi = i\hbar\frac{\partial\Psi}{\partial t} \tag{10}$$

where

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial t^2} + V. \tag{11}$$

To get the imaginary time Schrödinger equation make the substitution $\tau = it/\hbar$, or $t = -i\tau/\hbar$ to get

$$\hat{H}\Psi = -\frac{\partial\Psi}{\partial\tau}. \tag{12}$$

Notice that this is the diffusion equation (thus "diffusion" Monte Carlo), and thus the solutions to this consists of exponentials

$$\Psi(r,\tau) = \sum_{n=0}^{\infty} c_n\phi_n(r)e^{-\tau E_n}. \tag{13}$$

We now perform an energy shift to setting $V = V - E_0$ and $E_n = E_n - E_0$ to get

$$\Psi(r,\tau) = \sum_{n=0}^{\infty} c_n\phi_n(r)e^{-\tau(E_n-E_0)} \tag{14}$$

Now here is a key part, as you let $\tau \to \infty$ you get that $\Psi(r,\tau) \to \phi_0(r,\tau)$, which is the ground state wave function. This is because $E_n - E_0$ for $n > 0$ is a large number and essentially goes to zero.

$$\begin{aligned}\lim_{\tau\to\infty}\Psi(r,\tau) &= \lim_{\tau\to\infty}\sum_{n=0}^{\infty} c_n\phi_n(r)e^{-\tau(E_n-E_0)} \\ &= c_0\phi_0(r) + \lim_{\tau\to\infty}\sum_{n=1}^{\infty} c_n\phi_n(r)e^{-\tau(E_n-E_0)} \\ &= c_0\phi_0(r)\end{aligned} \tag{15}$$

To determine how to diffuse each walker and how to do the birth/death algorithm, lets look at the propagator (I'm just going to do the 1D case here) $|\psi(\tau)\rangle = e^{-(H-E_r)\tau}|\psi(0)\rangle$. The propagator, often called the Green's function, and is given by

$$\begin{aligned}\mathbf{G}(\mathbf{R}) &= \langle\mathbf{R}| e^{-(H-E_r)\tau} |\mathbf{R}'\rangle \\ &= \langle\mathbf{R}| e^{-(V-Er)\Delta\tau/2} e^{(\frac{p^2}{2m})\Delta\tau} e^{-(V-Er)\Delta\tau/2} |\mathbf{R}'\rangle \\ &= e^{-\Delta\tau(V(\mathbf{R})+V(\mathbf{R}')-2E_r)/2} \langle\mathbf{R}| e^{(\frac{p^2}{2m})\Delta\tau} |\mathbf{R}'\rangle .\end{aligned} \tag{16}$$

The part including the potential gives

$$P = \exp\left(-\Delta\tau\left(V(\mathbf{R}) + V(\mathbf{R}') - 2E_r\right)/2\right). \tag{17}$$

We need to take the Fourier trannsform of the kinetic part. This gives

$$\langle\mathbf{R}| \exp\left(-\frac{p^2\tau}{2m}\right) |\mathbf{R}'\rangle = \int_{-\infty}^{\infty} dp \, \langle\mathbf{R}|\mathbf{p}\rangle \exp\left(-\frac{p^2\tau}{2m}\right) \langle\mathbf{p}|\mathbf{R}'\rangle \tag{18}$$

$$= \int_{-\infty}^{\infty} dp \; e^{i\mathbf{p}\cdot\mathbf{R}} e^{-\frac{p^2\tau}{2m}} e^{-i\mathbf{p}\cdot\mathbf{R}'} \tag{19}$$

$$= \sqrt{\frac{2m\pi}{\tau}} \exp\left(-\frac{m(\mathbf{R}-\mathbf{R}')^2}{2\tau}\right) \tag{20}$$

Equation 17 is used to do the birth/death algorithm since it acts as a renormalization term and we sample from equation 20 to move the walkers at each step since it is the kinetic term.

## Procedure

The steps for performing DMC are shown below.

1. **Initialize:**
   (a) Randomly choose a distribution of walkers from some trial wave function $\Psi_T$.
   (b) The reference energy is set to something like the energy that you get from VMC, or the energy of the trial wave function.
2. **Imaginary time propagation**
   (a) Advance the time by $\Delta\tau$.
   (b) Move each walker according to Gaussian distribution with mean around the current walker and with standard deviation equal to

$$\sigma = \sqrt{\frac{\hbar\Delta\tau}{m}} \tag{21}$$

   (c) The reference energy is then reset to the value

$$E_{R,i} = E_{R,i-1} + \frac{\hbar}{\Delta\tau}\left(1 - \frac{N_i}{N_{i-1}}\right) \tag{22}$$

(d) The birth/death process is carried out. The integer part of the parameter $m$ is gives the number of walkers that process from 1 walker, where

$$m = \text{int}(P + \eta), \tag{23}$$

where $P$ is given by equation 17 and $\eta$ is drawn from a uniform distribution on $[0, 1]$. A maximum of two walkers can come from any walker [2].

3. The ground state is then given by the average of successive iterations of $E_R$. The ground state wave function is then given by the distribution of walkers (histogram).

## Importance Sampling

Importance sampling is used in [1] to improve the stability of DMC. This is done by multiplying the time dependent imaginary time schrödinger equation,

$$-\partial_t \Phi(\mathbf{R}, t) = (\hat{H} - E_T)\Phi(\mathbf{R}, t), \tag{24}$$

by $\Psi_T$ on both sides and define $f(\mathbf{R}, t) \equiv \Phi(\mathbf{R}, t)\Psi_T(\mathbf{R})$. This gives us

$$\begin{aligned}
-\partial_t f(\mathbf{R}, t) &= \Psi_T(\mathbf{R})\hat{H}\Phi(\mathbf{R}, t) - E_T f(\mathbf{R}, t) \\
&= -\Psi_T \frac{1}{2}\nabla^2\Phi + (V - E_T)f \\
&= -\frac{1}{2}\nabla^2 f + \frac{1}{2}\Phi\nabla^2\Psi_T + \frac{1}{2}2(\nabla\Phi)(\nabla\Psi_T) + \frac{1}{2}\Phi\nabla^2\Psi_T - \frac{1}{2}\Phi\nabla\Psi_T - E_T f + Vf \\
&= -\frac{1}{2}\nabla^2 f + \nabla\cdot(\Phi\nabla\Psi_T) - \frac{1}{2}\Phi\nabla^2\Psi_T - E_T f + Vf \\
-\partial_t f(\mathbf{R}, t) &= -\frac{1}{2}\nabla^2 f(\mathbf{R}, t) + \nabla\cdot(\mathbf{v_D} f(\mathbf{R}, t)) + (E_L - E_T)f(\mathbf{R}, t),
\end{aligned} \tag{25}$$

where I have used

$$\begin{aligned}
\nabla^2 f &= \Phi\nabla^2\Psi_T + \Psi_T\nabla^2\Phi + 2(\nabla\Phi)(\nabla\Psi_T) \\
\nabla\cdot(\Phi\nabla\Psi_T) &= (\nabla\Phi)(\nabla\Psi_T) + \Phi\nabla^2\Psi_T \\
\mathbf{V_D} &= \Psi_T^{-1}\nabla\Psi_T = \nabla\ln(\Psi_T) \\
E_L &= \Psi_T^{-1}\hat{H}\Psi_T = -\Psi_T^{-1}\frac{1}{2}\nabla^2\Psi_T + V.
\end{aligned} \tag{26}$$

Now the steps to do this method is described by [1] to be

1. Generate walkers from $|\Psi_T|^2$ distribution.
2. Calculate the local energies and $v_D$ for each walker.
3. Move each walker according to $\mathbf{R} = \mathbf{R}' + \chi + \Delta\tau\mathbf{v_D}(\mathbf{R}')$, where $\chi$ is drawn from a Gaussian with variance $\Delta\tau$ and zero mean.

4. If the trial wave function changes sign move it back to the original position.

5. Accept the step with probability

$$P_{\text{accept}}(\mathbf{R} \leftarrow \mathbf{R}') = \min\left[1, \frac{G_d(\mathbf{R}' \leftarrow \mathbf{R}, \Delta\tau)\Psi_T(\mathbf{R})^2}{G_d(\mathbf{R} \leftarrow \mathbf{R}', \Delta\tau)\Psi_T(\mathbf{R}')^2}\right] \tag{27}$$

where $G_d(\mathbf{R} \leftarrow \mathbf{R}', \Delta\tau)$ is given by

$$G_d(\mathbf{R} \leftarrow \mathbf{R}', \Delta\tau) = (2\pi\Delta\tau)^{-3N/2} \exp\left[-\frac{[\mathbf{R} - \mathbf{R}' - \Delta\tau \mathbf{v_D}(\mathbf{R}')]^2}{2\Delta\tau}\right] \tag{28}$$

6. Calculate how many walkers will come from each point using

$$M_{new} = \text{int}(\eta + \exp\{-\Delta\tau[E_L(\mathbf{R}) + E_L(\mathbf{R}') - 2E_T/2]\}), \tag{29}$$

where $\eta$ is drawn from a uniform distribution $[0, 1]$.

7. Accumulate the appropriate quantities to obtain the ground state energy and wave function.

The steps are then repeated until the ground state energy and wave function are projected out.

# Auxiliary Field Diffusion Monte Carlo

The methods described above are adequate for describing spin-independent potentials, but as described in [3] the number of spin-isospin states is

$$\frac{A!}{Z!(A-Z)!}2^A, \tag{30}$$

where $A$ is the nucleons and $Z$ is the number of protons, which is exponential in the number of particles. The number of states to be samples quickly becomes large. The AFDMC method is then used to simplify these methods.

My goal is to improve the trial function used in the current version of the code and so my comments will be directed toward this goal. The simplest trial wave function you can have is a slater determinant, which is the determinant of all of the single particle orbitals.

$$\Psi_T(\mathbf{r}) \doteq \begin{vmatrix} \phi_1(\mathbf{r_1}) & \phi_2(\mathbf{r_1}) & \cdots & \phi_N(\mathbf{r_1}) \\ \phi_1(\mathbf{r_2}) & \phi_2(\mathbf{r_2}) & \cdots & \phi_N(\mathbf{r_2}) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(\mathbf{r_N}) & \phi_2(\mathbf{r_N}) & \cdots & \phi_N(\mathbf{r_N}) \end{vmatrix} \tag{31}$$

This trial wave function does not include correlations. Ideally correlations would be included as

$$\langle \text{RS}|\Psi_T\rangle = \langle \text{RS}| \prod_{i<j} \left[ f_c(r_{ij}) \left[ 1 + \sum_{i<j,p} u_{ij}^p \mathcal{O}_{ij}^p \right] \right] |\Phi\rangle \,, \tag{32}$$

where the sum on $p$ in our code goes from 1 to 6, where the first 6 $\mathcal{O}_{ij}^p$ are 1, $\sigma_i \cdot \sigma_j$, $3\sigma_i \cdot \hat{r}_{ij}\sigma_j \cdot \hat{r}_{ij} - \sigma_i \cdot \sigma_j$, and the same things multiplied by $\tau_i \cdot \tau_j$. However, this requires too many operations. As discussed in [4] the correlations have currently been included as

$$\langle \mathrm{RS}|\Psi_T\rangle = \langle \mathrm{RS}| \left[\prod_{i<j} f_c(r_{ij})\right] \left[1 + \sum_{i<j,p} u_{ij}^p \mathcal{O}_{ij}^p\right] |\Phi\rangle \,. \tag{33}$$

This is a first approximation and does not include many terms in the interaction. The next step to move from equation 33 to equation 32 is to add the independent pair terms. This would look like

$$\langle \mathrm{RS}|\Psi_T\rangle = \langle \mathrm{RS}| \left[\prod_{i<j} f_c(r_{ij})\right] \left[1 + \sum_{i<j,p} u_{ij}^p \mathcal{O}_{ij}^p + \sum_{i<j,p}\sum_{k<l,p} u_{ij}^p \mathcal{O}_{ij}^p u_{kl}^p \mathcal{O}_{kl}^p\right] |\Phi\rangle \,. \tag{34}$$

I am currently working on understanding the code so that I can add these extra terms into the trial wave function.

Even though my project does not deal with the sampling of the spin states I will mention the idea here for completeness. As discussed in [3] the non-central part of the potential can be written in the form

$$V_{\mathrm{nc}} = \frac{1}{2}\sum_{n=1}^{3N} (O_n^{(\sigma)})^2 \lambda_n^{(\sigma)} + \frac{1}{2}\sum_{\alpha=1}^{3}\sum_{n=1}^{3N} (O_{n\alpha}^{(\sigma\tau)})^2 \lambda_n^{(\sigma\tau)} + \frac{1}{2}\sum_{\alpha=1}^{3}\sum_{n=1}^{N} (O_{n\alpha}^{(\tau)})^2 \lambda_n^{(\tau)}, \tag{35}$$

where the three squared operators are given by

$$\begin{aligned} O_n^{(\sigma)} &= \sum_i \boldsymbol{\sigma}_i \cdot \boldsymbol{\psi}_n^{(\tau)}(i) \\ O_{n\alpha}^{(\sigma\tau)} &= \sum_i \tau_{i\alpha} \boldsymbol{\sigma}_i \cdot \boldsymbol{\psi}_n^{(\sigma\tau)}(i) \\ O_{n\alpha}^{(\tau)} &= \sum_i \tau_{i\alpha} \psi_n^{(\tau)}(i), \end{aligned} \tag{36}$$

where the $\psi$'s are the eigenfunctions of symmetric matrices that consist of phenomenological data. At this point the Hubbard-Stratonovich transformation can be used to take these squared operators and convert them to linear operators using the equation

$$e^{-\frac{1}{2}\lambda_n O_n^2 \Delta t} = \left(\frac{\Delta t|\lambda_n|}{2\pi}\right)^{1/2} \int_{-\infty}^{\infty} dx e^{-\frac{1}{2}\Delta t|\lambda_n|x^2 - \Delta t s \lambda_n O_n x}. \tag{37}$$

Notice how the $O_n$ term goes from quadratic to linear. This transformation is what gives the method the name Auxiliary Field.

# References


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