

Report on Research Rotation I

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Abstract

I have learned how to use Variational Monte Carlo (VMC) and Diffusion Monte Carlo (DMC) methods to solve the Schrödinger equation for simple systems. I have applied these methods to both 1D and 3D harmonic oscillators, as well as systems with x^4 potentials. I was able to verify that my results agreed with the exact results for the harmonic oscillator systems. I have learned the basics of Auxiliary Field Diffusion Monte Carlo (AFDMC) and have described the additions that I plan to make to the existing AFDMC code.

Introduction

Solving the Schrödinger equation for many-body nuclear systems gets difficult as the number of particles increases and as the potential term in the Hamiltonian gets more complicated. To overcome this we can use Monte Carlo methods. These methods require a good nuclear Hamiltonian and a good trial wave function. One of the things that makes it difficult to get a good nuclear Hamiltonian is the spin dependence. Another thing that makes them difficult to obtain is the little understanding that we have of the strong nuclear force, which is responsible for the binding together of quarks to form nucleons as well as binding nucleons together to form nuclei. Since we cannot come up with exact expressions for these strong force interactions we use phenomenological methods to obtain the potentials. The usual Hamiltonians come from the Argonne and Urbana potentials [1, 2]. The Hamiltonians that we use are of the form

$$H = \sum_{i=1}^A \frac{\mathbf{p}_i^2}{2m} + V, \quad (1)$$

where V takes the form

$$V = \sum_{i < j}^A \sum_p v_p(r_{ij}) \mathcal{O}_{ij}^{(p)}. \quad (2)$$

For our purposes p will run from 1 – 6 and the $\mathcal{O}^{(p)}$ are given by 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 $\tau_i \cdot \tau_j$. More detail can be found in [3]. This Hamiltonian is then used in the Schrödinger equation

$$i \frac{\partial \Psi(R, S, t)}{\partial t} = H \Psi(R, S, t) \quad (3)$$

to solve for the ground state energy and wavefunction for particular nuclear systems. The two nuclear systems that we typically study are atomic nuclei and nuclear matter.

In preparation for using and modifying the current Auxiliary Field Diffusion Monte Carlo (AFDMC) code [3, 4] I have used Variational Monte Carlo (VMC) and Diffusion Monte Carlo (DMC) as described in [5, 6] to solve the quantum harmonic oscillator (QHO) and the similar problem with an x^4 potential. I will first describe these two Monte Carlo methods in a general form, and then I will apply the DMC method to the QHO.

Variational Monte Carlo

There are many good books that describe the basics of the VMC method, but I found the explanation in [5] 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

$$I = \int g(\mathbf{R}) d\mathbf{R}. \quad (4)$$

This can be rewritten as

$$I = \int f(\mathbf{R}) P(\mathbf{R}) d\mathbf{R} \quad (5)$$

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 $\mathbf{R} = (\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_n)$, where \mathbf{r}_i is the position of the i th 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 $\langle \hat{H} \rangle = \int_{-\infty}^{\infty} \langle \psi | \hat{H} | \psi \rangle$).

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

$$I = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N f(\mathbf{R}_n) \quad (6)$$

The integral can then be approximated by

$$I \approx \frac{1}{N} \sum_{n=1}^N f(\mathbf{R}_n). \quad (7)$$

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

$$A(\mathbf{R}' \leftarrow \mathbf{R}) = \min \left(1, \frac{T(\mathbf{R}' \leftarrow \mathbf{R})P(\mathbf{R}')} {T(\mathbf{R} \leftarrow \mathbf{R}')P(\mathbf{R})} \right). \quad (8)$$

$T(\mathbf{R}' \leftarrow \mathbf{R})$ 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 trial wave function Ψ_T . The accuracy of VMC is sensitive to the choice of Ψ_T . The trial wave function is then used to find a rigid upper bound on the ground state energy, E_0 .

$$E_V = \frac{\int \Psi_T^*(\mathbf{R}) \hat{H} \Psi_T(\mathbf{R}) d\mathbf{R}}{\int \Psi_T^*(\mathbf{R}) \Psi_T(\mathbf{R}) d\mathbf{R}} \leq E_0 \quad (9)$$

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

$$E_V = \frac{\int |\Psi_T(\mathbf{R})|^2 [\Psi_T^{-1}(\mathbf{R}) \hat{H} \Psi_T(\mathbf{R}) d\mathbf{R}]}{\int |\Psi_T(\mathbf{R})|^2 d\mathbf{R}}. \quad (10)$$

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

$$E_V = \int P(\mathbf{R}) E_L(\mathbf{R}) d\mathbf{R}. \quad (11)$$

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

$$E_V \approx \frac{1}{N} \sum_{n=1}^N E_L(\mathbf{R}_n). \quad (12)$$

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

Diffusion Monte Carlo

This explanation also draws heavily from [5], but also draws a good deal from [6]. The time dependent Schrödinger equation is

$$\hat{H}\Psi = i\hbar \frac{\partial \Psi}{\partial t} \quad (13)$$

where

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial t^2} + V. \quad (14)$$

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

$$\hat{H}\Psi = -\frac{\partial \Psi}{\partial \tau}. \quad (15)$$

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

$$\Psi(r, \tau) = \sum_{n=0}^{\infty} c_n \phi_n(r, \tau) e^{-\tau E_n}. \quad (16)$$

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

$$\Psi(r, \tau) = \sum_{n=0}^{\infty} c_n \phi_n(r, \tau) e^{-\tau(E_n - E_0)} \quad (17)$$

Now here is a key part, as you let $\tau \rightarrow \infty$ you get that $\Psi(r, \tau) \rightarrow \Psi_0(r, \tau)$, 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.

$$\begin{aligned} \lim_{\tau \rightarrow \infty} \Psi(r, \tau) &= \lim_{\tau \rightarrow \infty} \sum_{n=0}^{\infty} c_n \phi_n(r, \tau) e^{-\tau(E_n - E_0)} \\ &= c_0 \phi_0(r, \tau) + \lim_{\tau \rightarrow \infty} \sum_{n=1}^{\infty} c_n \phi_n(r, \tau) e^{-\tau(E_n - E_0)} \\ &= c_0 \phi_0(r) \end{aligned} \quad (18)$$

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

$$\begin{aligned} \mathbf{G}(x) &= \langle x | e^{-(H-E_r)\tau} | x' \rangle \\ &= \langle x | e^{-(V-E_r)\Delta\tau/2} e^{(\frac{p^2}{2m})\Delta\tau} e^{-(V-E_r)\Delta\tau/2} | x \rangle \\ &= e^{-\Delta\tau(V(x)+V(x')-2E_r)/2} \langle x | e^{(\frac{p^2}{2m})\Delta\tau} | x' \rangle. \end{aligned} \quad (19)$$

Now do a Fourier transform on the kinetic part to get it in terms of x and you get the two parts,

$$\exp(-\Delta\tau (V(x) + V(x') - 2E_r) / 2) \quad (20)$$

$$\exp(-\frac{mx^2}{2\Delta\tau}) \quad (21)$$

Equation 20 is used to do the birth/death algorithm and we sample from equation 21 to move the walkers at each step.

Procedure

The steps for performing DMC are shown below.

1. Initialize:

- (a) Randomly choose a distribution of walkers from some trial wave function Ψ_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

$$\sigma = \sqrt{\frac{\hbar\Delta\tau}{m}} \quad (22)$$

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

$$E_{R,i} = E_{R,i-1} + \frac{\hbar}{\Delta\tau} \left(1 - \frac{N_i}{N_{i-1}} \right) \quad (23)$$

- (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

$$m = \text{int}(W(r) + U), \quad (24)$$

where $W(r)$ is given by

$$W(r) = e^{-\Delta\tau((V(r_i)+V(r_{i-1}))/2-E_R)/\hbar}. \quad (25)$$

A maximum of two walkers can come from any walker [6].

- 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 [5] to improve the stability of DMC. This is done by multiplying the time dependent imaginary time schrödinger equation,

$$-\partial_t \Phi(\mathbf{R}, t) = (\hat{H} - E_T) \Phi(\mathbf{R}, t), \quad (26)$$

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

$$\begin{aligned} -\partial_t f(\mathbf{R}, t) &= \Psi_T(\mathbf{R}) \hat{H} \Phi(\mathbf{R}, t) - E_T f(\mathbf{R}, t) \\ &= -\Psi_T \frac{1}{2} \nabla^2 \Phi + (V - E_T) f \\ &= -\frac{1}{2} \nabla^2 f + \frac{1}{2} \Phi \nabla^2 \Psi_T + \frac{1}{2} 2(\nabla \Phi)(\nabla \Psi_T) + \frac{1}{2} \Phi \nabla^2 \Psi_T - \frac{1}{2} \Phi \nabla \Psi_T - E_T f + V f \\ &= -\frac{1}{2} \nabla^2 f + \nabla \cdot (\Phi \nabla \Psi_T) - \frac{1}{2} \Phi \nabla^2 \Psi_T - E_T f + V f \\ -\partial_t f(\mathbf{R}, t) &= -\frac{1}{2} \nabla^2 f(\mathbf{R}, t) + \nabla \cdot (\mathbf{v}_D f(\mathbf{R}, t)) + (E_L - E_T) f(\mathbf{R}, t), \end{aligned} \quad (27)$$

where I have used

$$\begin{aligned}
\nabla^2 f &= \Phi \nabla^2 \Psi_T + \Psi_T \nabla^2 \Phi + 2(\nabla \Phi)(\nabla \Psi_T) \\
\nabla \cdot (\Phi \nabla \Psi_T) &= (\nabla \Phi)(\nabla \Psi_T) + \Phi \nabla^2 \Psi_T \\
\mathbf{V}_D &= \Psi_T^{-1} \nabla \Psi_T = \nabla \ln(\Psi_T) \\
E_L &= \Psi_T^{-1} \hat{H} \Psi_T = -\Psi_T^{-1} \frac{1}{2} \nabla^2 \Psi_T + V.
\end{aligned} \tag{28}$$

Now the steps to do this method is described by [5] 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 χ 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

$$P_{\text{accept}}(\mathbf{R} \leftarrow \mathbf{R}') = \min \left[1, \frac{G_d(\mathbf{R}' \leftarrow \mathbf{R}, \Delta\tau) \Psi_T(\mathbf{R})^2}{G_d(\mathbf{R} \leftarrow \mathbf{R}', \Delta\tau) \Psi_T(\mathbf{R}')^2} \right] \tag{29}$$

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

$$G_d(\mathbf{R} \leftarrow \mathbf{R}', \Delta\tau) = (2\pi\Delta\tau)^{-3N/2} \exp \left[-\frac{[\mathbf{R} - \mathbf{R}' - \Delta\tau \mathbf{v}_D(\mathbf{R}')]^2}{2\Delta\tau} \right] \tag{30}$$

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

$$M_{\text{new}} = \text{int}(\eta + \exp \{ -\Delta\tau [E_L(\mathbf{R}) + E_L(\mathbf{R}') - 2E_T/2] \}), \tag{31}$$

where η 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.

Quantum Harmonic Oscillator with DMC

First of all the Hamiltonian is given by (Assuming 1D for simplicity, but it can be easily modified for 3D)

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} m \omega^2 x^2. \tag{32}$$

Using natural units where $\hbar = 1, \omega = 1, m = 1$ and energy is measured in units of $\hbar\omega$, this gives

$$\hat{H} = -\frac{1}{2} \frac{\partial^2}{\partial x^2} + \frac{1}{2} x^2. \tag{33}$$

Since I know the answer I can use the exact wave function as my trial wave function.

$$\Psi_T(x) = \pi^{-1/4} \exp\left(-\frac{x^2}{2}\right) \quad (34)$$

Using the above equations this gives us

$$\begin{aligned} v_D &= \Psi_T^{-1} \frac{\partial}{\partial x} \Psi_T = -x \\ E_L &= \Psi_T^{-1} \hat{H} \Psi_T = \frac{1}{2} \end{aligned} \quad (35)$$

Figure 1 shows the results for a DMC calculation of a 1-d harmonic oscillator. The exact energy for the 1-d oscillator is $E = \frac{1}{2}\hbar\omega$. The DMC energy for the calculation described in figure 1 was $E = 0.49\hbar\omega$. I also did a calculation for a particle in a

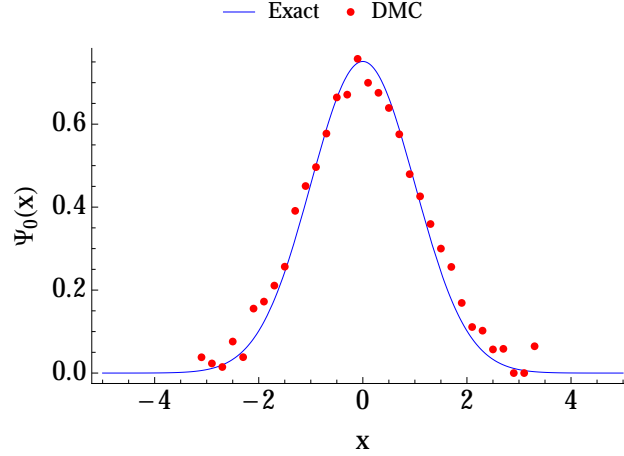


Figure 1: DMC results for 1-d harmonic oscillator. Number of initial walkers was 10000, time step was 0.01, and number of time steps was 500. The exact energy is $E = \frac{1}{2}\hbar\omega$ and the DMC energy was $E = 0.49\hbar\omega$.

potential $V(x) = \frac{1}{2}x^4$, using the exact solution for the harmonic oscillator as the trial wave function. The DMC energy for this calculation was $E = 0.57\hbar\omega$, and the resulting ground state wave function is shown in figure 2.

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

$$\frac{A!}{Z!(A-Z)!} 2^A, \quad (36)$$

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.

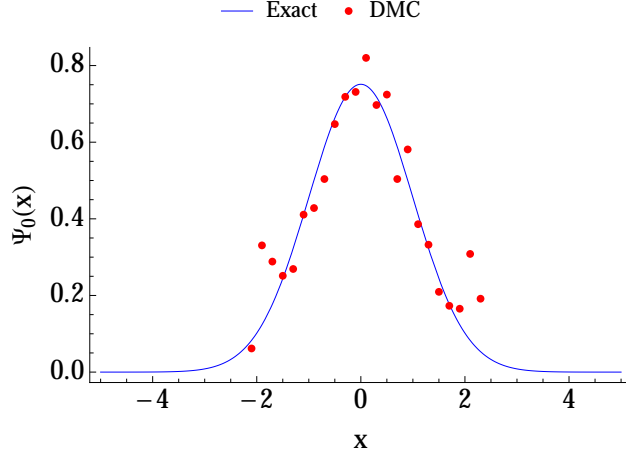


Figure 2: DMC results for particle in an x^4 potential. Number of initial walkers was 1000, time step was 0.01, and number of time steps was 500. The DMC energy was $E = 0.57\hbar\omega$. The exact solution in this case represents the exact solution for the quantum harmonic oscillator.

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.

$$\Psi_T(\mathbf{r}) \doteq \begin{vmatrix} \phi_1(\mathbf{r}_1) & \phi_2(\mathbf{r}_1) & \cdots & \phi_N(\mathbf{r}_1) \\ \phi_1(\mathbf{r}_2) & \phi_2(\mathbf{r}_2) & \cdots & \phi_N(\mathbf{r}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(\mathbf{r}_N) & \phi_2(\mathbf{r}_N) & \cdots & \phi_N(\mathbf{r}_N) \end{vmatrix} \quad (37)$$

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

$$\langle \text{RS} | \Psi_T \rangle = \langle \text{RS} | \prod_{i < j} \left[f_c(r_{ij}) \left[1 + \sum_{i < j, p} u_{ij}^p \mathcal{O}_{ij}^p \right] \right] | \Phi \rangle, \quad (38)$$

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

$$\langle \text{RS} | \Psi_T \rangle = \langle \text{RS} | \left[\prod_{i < j} f_c(r_{ij}) \right] \left[1 + \sum_{i < j, p} u_{ij}^p \mathcal{O}_{ij}^p \right] | \Phi \rangle. \quad (39)$$

This is a first approximation and does not include many terms in the interaction. The next step to move from equation 39 to equation 38 is to add the independent pair terms. This would look like

$$\langle \text{RS} | \Psi_T \rangle = \langle \text{RS} | \left[\prod_{i < j} f_c(r_{ij}) \right] \left[1 + \sum_{i < j, p} u_{ij}^p \mathcal{O}_{ij}^p + \sum_{i < j, p} \sum_{k < l, p} u_{ij}^p \mathcal{O}_{ij}^p u_{kl}^p \mathcal{O}_{kl}^p \right] | \Phi \rangle. \quad (40)$$

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

$$V_{\text{nc}} = \frac{1}{2} \sum_{n=1}^{3N} (O_n^{(\sigma)})^2 \lambda_n^{(\sigma)} + \frac{1}{2} \sum_{\alpha=1}^3 \sum_{n=1}^{3N} (O_{n\alpha}^{(\sigma\tau)})^2 \lambda_n^{(\sigma\tau)} + \frac{1}{2} \sum_{\alpha=1}^3 \sum_{n=1}^N (O_{n\alpha}^{(\tau)})^2 \lambda_n^{(\tau)}, \quad (41)$$

where the three squared operators are given by

$$\begin{aligned} O_n^{(\sigma)} &= \sum_i \boldsymbol{\sigma}_i \cdot \boldsymbol{\psi}_n^{(\sigma)}(i) \\ O_{n\alpha}^{(\sigma\tau)} &= \sum_i \tau_{i\alpha} \boldsymbol{\sigma}_i \cdot \boldsymbol{\psi}_n^{(\sigma\tau)}(i) \\ O_{n\alpha}^{(\tau)} &= \sum_i \tau_{i\alpha} \psi_n^{(\tau)}(i), \end{aligned} \quad (42)$$

where the ψ '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

$$e^{-\frac{1}{2} \lambda_n O_n^2 \Delta t} = \left(\frac{\Delta t |\lambda_n|}{2\pi} \right)^{1/2} \int_{-\infty}^{\infty} dx e^{-\frac{1}{2} \Delta t |\lambda_n| x^2 - \Delta t \lambda_n O_n x}. \quad (43)$$

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

Conclusion

In conclusion, I have learned how to implement VMC and DMC methods and have applied these methods to the quantum harmonic oscillator as well as a similar x^4 potential. The ground state energies and wave functions that I obtained were close to the exact solutions for the harmonic oscillator. I have also learned the basics of the AFDMC method and have been working on understanding the existing code. Further work will include the addition of the extra terms in the trial wave function correlations. These additions will then be compared to the existing code for a variety of nuclear systems.

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