Auxiliary Field Quantum Monte Carlo (AFQMC) Exercises

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These exercises are designed to familiarize you with Auxiliary Field Quantum Monte Carlo (AFQMC), a type of Quantum Monte Carlo that works in the space of Slater determinants and stochastically samples wave functions by sampling sets of auxiliary fields (see References below for more details). Here, we will focus on applying AFQMC to a simple Hubbard model to illustrate the basic ideas and components of the algorithm. It should be noted that when Hubbard-Stratonovich Transformations that yield only real propagators are required and only constraints on the sign are employed, AFQMC is commonly called Constrained Path Monte Carlo (CPMC). Both terms will be used to describe the methods below.

1 CONSTRUCTING ONE-BODY OPERATORS AND THEIR WAVE FUNCTIONS FOR THE 4-SITE HUBBARD MODEL

1.1 THE HUBBARD MODEL

The simplest Hamiltonian for studying strong correlation is the Hubbard Hamiltonian

$$\hat{H}_{Hubbard} = \hat{K} + \hat{V} = -t \sum_{\langle ij \rangle, \sigma} \left(\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \hat{c}^{\dagger}_{j\sigma} \hat{c}_{i\sigma} \right) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}, \tag{1.1}$$

where $\hat{c}^{\dagger}_{i\sigma}$ is a creation operator that creates an electron at site i with spin σ, $\hat{c}_{j\sigma}$ is the corresponding annihilation operator that destroys an electron on site j with spin σ, $\hat{n}_{i\uparrow} = \hat{c}^{\dagger}_{i\uparrow} \hat{c}_{i\uparrow}$ denotes the number of spin-up electrons on site i, t is the hopping constant, and U is the interaction constant. Note that $\hat{K}$ denotes the kinetic (one-body) portion of the Hamiltonian,

while $\hat{V}$ denotes the potential (two-body) portion of the Hamiltonian. The Hubbard Hamiltonian illustrates the competition between electron delocalization (via the hopping terms) and electron repulsion (via the interaction term) to yield the lowest possible system energy.

1.2 Constructing One-Body Operators

In order to acquaint you with both the Hubbard model and working with second-quantized Hamiltonians, for your first task, consider how you would construct the one-body operator, $\hat{K}$, for the 4-site, 1-dimensional Hubbard model with periodic boundary conditions. One-body operators can be written down as matrices.

1.2.1 Exercises

1. What would the $\hat{K}$ matrix look like in this case? Program a way to obtain the $\hat{K}$ matrices for the 1D, Hubbard model with an arbitrary number of sites under periodic boundary conditions (if you can't think of a general way, you can hard code the 4-site case for now).

2. How would the $\hat{K}$ matrix change if we chose to use open or anti-periodic boundary conditions instead?

3. *(Advanced)* How could the $\hat{K}$ matrix be generalized to handle molecular one-body interactions? What would the *ab initio* one-body matrix look like? How are the one-body molecular constants that correspond to t here obtained? To what do they correspond?

Once you are confident in your $\hat{K}$ matrix, consider how to obtain non-interacting solutions to the Hubbard model for varying numbers of spin-up and spin-down electrons. The non-interacting solution is useful because: a) it provides us with a benchmark against which we compare small-U QMC results and b) AFQMC simulations often use non-interacting wave functions as their trial wave functions.

1.2.2 Exercises

1. How can you obtain the non-interacting solutions (both energies and wave functions) to this Hubbard model from $\hat{K}$? Program this into your code.

2. What would be the non-interacting wave function if our model contains 2 up and 3 down electrons? 1 up and 4 down electrons? What changes about the wave function as the number of electrons is varied?

3. *(General Considerations)* What is the scaling involved with finding non-interacting solutions? Why does this make manipulating $\hat{K}$ particularly convenient compared with manipulating $\hat{H}$?

2 Propagation in AFQMC

2.1 Propagating the Non-Interacting Hamiltonian Wave Function

At its core, AFQMC is a projector QMC technique, which means that it relies upon iteratively projecting upon a trial wave function to eventually obtain the ground state wave function

$$|\Psi_G\rangle = \lim_{n\to\infty}\left(e^{-\Delta\tau\hat{H}}\right)^n |\Psi_{Trial}\rangle, \tag{2.1}$$

where $|\Psi_{Trial}\rangle$ is the trial wave function (which could be the non-interacting wave function, as above), $|\Psi_G\rangle$ denotes the ground state wave function, $\Delta\tau$ is the time slice, and n is the number of iterations. A basic part of performing AFQMC is therefore understanding how to iteratively propagate a given wave function

$$|\Psi^{(n+1)}\rangle = e^{-\Delta\tau\hat{H}}|\Psi^{(n)}\rangle. \tag{2.2}$$

2.1.1 Exercises

For simplicity, let's assume that $\hat{V} = 0$ and that $\hat{H} = \hat{K}$.

1. How can $e^{-\Delta\tau\hat{K}}$ be obtained for arbitrary $\Delta\tau$? Program this into your code.
2. Once you obtain a form for $e^{-\Delta\tau\hat{K}}$, create a loop in your code that applies this operator iteratively to the wave function. This is the core loop in AFQMC.
3. Print out your wave function after each iteration. How can you tell if you are converged? What would be the best property to measure in order to tell if you have converged?

2.2 *(Advanced)* Measuring the Energy

In order to measure the energy, we must evaluate

$$\langle E\rangle = \frac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle}. \tag{2.3}$$

In QMC simulations, we often simplify the computational task required to obtain $\langle E\rangle$ by obtaining the mixed estimator, $\langle E_{mixed}\rangle$, instead

$$\langle E_{mixed}\rangle = \frac{\langle\Psi_T|\hat{H}|\Psi\rangle}{\langle\Psi_T|\Psi\rangle}. \tag{2.4}$$

For the non-orthogonal determinants produced in AFQMC, this expression may be simplified by noting that

$$\langle\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\rangle = \frac{\langle\Psi_T|\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}|\Psi\rangle}{\langle\Psi_T|\Psi\rangle} \tag{2.5}$$

$$= \left[\Psi^\sigma\left[\left(\Psi^\sigma_T\right)^\dagger\Psi^\sigma\right]^{-1}(\Psi_T)^\dagger\right]_{ij}. \tag{2.6}$$

For the non-interacting case, it is easy to see that

$$\langle E\rangle_{mixed} = \frac{\langle\Psi_T|\hat{K}|\Psi\rangle}{\langle\Psi_T|\Psi\rangle} \tag{2.7}$$

$$= -t\sum_{\langle ij\rangle\sigma}\frac{\langle\Psi_T|\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}+\hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}|\Psi\rangle}{\langle\Psi_T|\Psi\rangle} \tag{2.8}$$

$$= -t\sum_{\langle ij\rangle\sigma}\left(\langle\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\rangle+\langle\hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}\rangle\right). \tag{2.9}$$

2.2.1 Exercises

1. Given these expressions, calculate the mixed estimator of the non-interacting energy.
2. Print out this energy estimator after each iteration to track the convergence of the energy in your simulation.

3 The Potential and the Hubbard-Stratonovich (HS) Transformation

Thus far, we have focused on the non-interacting Hamiltonian. This is because the non-interacting Hamiltonian is a one-body operator and the exponential of a one-body operator can be written as a matrix. The same is not true for two-body operators. Exponentials of two-body operators must therefore be converted into exponentials of one-body operators. This is achieved via the Hubbard-Stratonovich Transformation (HS).

3.1 The Scalar Hubbard-Stratonovich Transformation

The Hubbard-Stratonovich Transformation is based upon rearranging the usual shifted-Gaussian integral

$$1 = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-1/2(x\pm y)^2}\,dx. \tag{3.1}$$

An expression for $e^{y^2/2}$ (an exponential of a square, which is what we need to evaluate $e^{-\Delta\tau\hat{V}}$) simply requires rearranging this expression

$$e^{y^2/2} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-1/2(x^2\pm 2xy)}\,dx. \tag{3.2}$$

Note that this expression looks exactly like the integral of a Gaussian. What this implies is that $e^{y^2/2}$ can be obtained by sampling a Gaussian distribution for x, what we term our "auxiliary field," and using x to collect samples of e^{-xy}.

3.1.1 EXERCISES

1. For an arbitrary value of y, develop a program that computes $e^{y^2/2}$ using the Hubbard-Stratonovich Transformation. This should involve sampling a Gaussian distribution for the x's, using those x's to evaluate e^{-xy}, and then averaging over those samples to obtain your final result. Feel free to use software from Day 1 to help with sampling and averaging.

3.2 THE OPERATOR HUBBARD-STRATONOVICH TRANSFORMATION

The continuous Hubbard-Stratonovich Transformation (continuous because x can assume any real value) is readily translated into operator form

$$e^{-(\Delta\tau/2)\lambda\hat{v}^2} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx e^{-x^2/2} e^{x\sqrt{-\Delta\tau\lambda}\hat{v}}, \tag{3.3}$$

where $\hat{v}$ denotes a one-body operator, x is an auxiliary field just like before, and λ is a constant. This was obtained from Equation 3.2 by letting $y = \sqrt{-\Delta\tau\lambda}\hat{v}$. What this equation implies is that, as long as a two-body operator may be written as the sum of squares, it can be evaluated by sampling a Gaussian-distribution of one-body operators. This is where the stochastic nature of AFQMC comes into play.

To see how the HS Transformation can be used on the Hubbard Model, we must rewrite the propagator. In order to use Equation 2.1 for the full Hamiltonian, in AFQMC, we make use of the Suzuki-Trotter factorization to break the exponential of the Hamiltonian into kinetic and potential pieces

$$e^{-\Delta\tau\hat{H}} \approx e^{-\Delta\tau\hat{K}/2} e^{-\Delta\tau\hat{V}} e^{-\Delta\tau\hat{K}/2}, \tag{3.4}$$

which holds only for a sufficiently small $\Delta\tau$. The one-body exponentials may be evaluated as in the previous exercises. We now turn to how to evaluate the potential piece, $e^{-\Delta\tau\hat{V}}$. For the Hubbard model,

$$\begin{aligned} e^{-\Delta\tau\hat{V}} &= e^{-\Delta\tau U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}} && (3.5)\\ &= \prod_i e^{-\Delta\tau U\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}}. && (3.6) \end{aligned}$$

In order to use the HS Transformation, this needs to be cast into an exponential of squares of densities. This may be done by recognizing (using operator algebra) that

$$\hat{n}_\uparrow\hat{n}_\downarrow = -\frac{(\hat{n}_\uparrow - \hat{n}_\downarrow)^2}{2} + \frac{(\hat{n}_\uparrow + \hat{n}_\downarrow)}{2}. \tag{3.7}$$

Substituting this into Equation 3.6 yields

$$e^{-\Delta\tau\hat{V}} = \prod_i e^{\Delta\tau U(\hat{n}_{i\uparrow}-\hat{n}_{i\downarrow})^2/2} e^{-\Delta\tau U(\hat{n}_{i\uparrow}+\hat{n}_{i\downarrow})/2}. \tag{3.8}$$

Substituting the exponential of the squared term with the HS Transformation produces the final result

$$e^{-\Delta\tau\hat{V}} = \prod_i e^{-\Delta\tau U(\hat{n}_{i\uparrow}+\hat{n}_{i\downarrow})/2} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx_i e^{-x_i^2/2} e^{x_i\sqrt{\Delta\tau U}(\hat{n}_{i\uparrow}-\hat{n}_{i\downarrow})}. \tag{3.9}$$

3.2.1 Exercises

1. Use operator algebra to demonstrate the validity of Equation 3.7.
2. Given a particular auxiliary field, x_i, how would you construct the one-body propagator $e^{x_i\sqrt{\Delta\tau U}(\hat{n}_{i\uparrow}-\hat{n}_{i\downarrow})}$ on site i? What would you have to do with the different spin components? How could you deal with the $e^{-\Delta\tau U(\hat{n}_{i\uparrow}+\hat{n}_{i\downarrow})/2}$ term?
3. What would be the result of the HS transform if the decomposition $\hat{n}_\uparrow\hat{n}_\downarrow = (\hat{n}_\uparrow+\hat{n}_\downarrow)^2/2 - (\hat{n}_\uparrow+\hat{n}_\downarrow)/2$ was used instead? What happens to the propagator? This relates to the origin of the phase problem.
4. *(Advanced)* Perform and code the Hubbard-Stratonovich Transformation given by Equation 3.9 by sampling Gaussian-distributed fields at each site i and evaluating the corresponding one-body operators. How would $e^{-\Delta\tau\hat{V}}|\Psi_T\rangle$ be performed?

4 Illustrative AFQMC Simulation

Based upon your previous work constructing one-body propagators and performing HS transformations, the last ingredient for a basic (without importance sampling, population control, orthogonalization, etc.) AFQMC algorithm is to integrate the HS transformation into your propagation loop from your previous exercises.

4.1 Implementing the AFQMC Inner Propagation Loop

As mentioned before, the basic iteration required in AFQMC is

$$\begin{aligned}
|\Psi^{(n+1)}\rangle &= e^{-\Delta\tau\hat{H}}|\Psi^{(n)}\rangle && (4.1)\\
&\approx e^{-\Delta\tau\hat{K}/2}e^{-\Delta\tau\hat{V}}e^{-\Delta\tau\hat{K}/2}|\Psi^{(n)}\rangle && (4.2)\\
&= e^{-\Delta\tau\hat{K}/2}\left[\prod_i e^{-\Delta\tau U(\hat{n}_{i\uparrow}+\hat{n}_{i\downarrow})/2}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx_i e^{-x_i^2/2} e^{x_i\sqrt{\Delta\tau U}(\hat{n}_{i\uparrow}-\hat{n}_{i\downarrow})}\right] e^{-\Delta\tau\hat{K}/2}|\Psi^{(n)}\rangle. && (4.3)
\end{aligned}$$

4.1.1 Exercises

1. Evaluate the one-body $e^{-\Delta\tau\hat{K}/2}$ operators. Note the factor of 1/2.
2. Iteratively multiply your previous wave function by $e^{-\Delta\tau\hat{K}/2}$, the HS form for $e^{-\Delta\tau\hat{V}}$, and $e^{-\Delta\tau\hat{K}/2}$. This loop is your full AFQMC loop.

3. *(Advanced)* Use the energy calculator you wrote to evaluate the mixed estimator for the energy every so many AFQMC iterations. How would you evaluate the average potential energy term? Plot the energy as a function of imaginary time (number of iterations). Observe the fluctuations.

4.2 Weighting and Walkers

This is a school on stochastic electronic structure, so you may be wondering where weights come into play in this algorithm. So far, you have worked on propagating single walkers. To perform a random walk through Slater determinant space, we create a set of walkers, k, which are each represented by the structure $\{\Psi_k, w_k, \theta_k\}$, where Ψ_k denotes walker k's Slater determinant, w_k denotes its real and positive weight, and θ_k denotes its phase angle. Note that, altogether, the weight of a walker, including any imaginary contributions that may emerge from complex Hubbard-Statronovich Transformations, is $w_k e^{i\theta_k}$. At the beginning of a simulation, we initialize each walker to start at some initial wave function, which can be a non-interacting trial wave function, with weight 1 and phase angle 0. Then, as the simulation progresses, we sample each auxiliary field and update each walker's Slater determinants as described above

$$|\Psi_k^{n+1}\rangle = \hat{B}(\vec{x}_k^{n+1})|\Psi_k^n\rangle, \tag{4.4}$$

but also update their weights as

$$w_k^{n+1} e^{i\theta_k^{n+1}} = \frac{\langle \Psi_T|\Psi_k^{n+1}\rangle}{\langle \Psi_T|\Psi_k^n\rangle} w_k^n e^{i\theta_k^n}. \tag{4.5}$$

Thus, every time we advance a walker, we determine the ratio of its current Slater determinant's overlap with the initial wave function and its previous Slater determinant's overlap and update its weight by this factor. After some amount of propagation, when we desire estimates of the ground-state energy, we then weight the local energy contributions from each walker

$$\langle E_{mixed}\rangle \approx \frac{\sum_k w_k e^{i\theta_k} E_{loc}(\Psi_k)}{\sum_k w_k e^{i\theta_k}}, \tag{4.6}$$

where

$$E_{loc}(\Psi_k) = \frac{\langle \Psi_T|\hat{H}|\Psi_k\rangle}{\langle \Psi_T|\Psi_k\rangle}, \tag{4.7}$$

as in Equations 2.4, 2.6, 2.5, 2.7, and 2.8.

4.2.1 Exercises

1. Attempt to implement the full kinetic and potential propagation for a large number of walkers. What do you expect to happen to the accuracy of your results as you increase the number of walkers? *And, how would you check this?*

2. *(Advanced)* During the course of this summer school, you should have learned population control techniques for controlling walker weights. Which techniques could be used in this context? If you have the opportunity, implement one of them and note any changes to your answers.

4.3 Future Thoughts

1. (***Ab Initio* Hamiltonians)** We have thus far focused on the Hubbard Model. What would change when simulating a fully *ab initio* Hamiltonian? What form does such a Hamiltonian take in second-quantization? What form would your Hubbard-Stratonovich Transformation assume? We will discuss this during our concluding conversations. Feel free to also peruse the following references if you are unsure/interested.

2. (**Constraints)** We have not had the opportunity to explore how to implement the trial wave function-based constraints, including the constrained path and phaseless approximation, that are essential for polynomial-scaling AFQMC simulations. Please also see the references below for a full discussion.

5 References

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