Auxiliary Field Quantum Monte Carlo (AFQMC) Exercise Solutions

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

1.0.1 EXERCISE SOLUTIONS

1. For a 4-site, 1D Hubbard Model with periodic boundary conditions, the hopping terms will connect site 1 with sites 2 and 4, site 2 with sites 1 and 3, site 3 with sites 2 and 4, and site 4 with sites 3 and 1. This leads to the matrix

$$\hat{K} = \begin{bmatrix} 0 & -t & 0 & -t \\ -t & 0 & -t & 0 \\ 0 & -t & 0 & -t \\ -t & 0 & -t & 0 \end{bmatrix}. \tag{1.1}$$

   Generalizations of this should place a hopping constant at sites immediately less than and greater than a given site, creating a banded matrix. Exceptions must be made for the first and last sites at the edges of the lattice sot that the corresponding electrons periodically hop to the opposite edges of the lattice.

2. Open boundary conditions would imply that electrons cannot hop around the bound-

aries. This would imply that the corresponding $-t$'s become 0

$$\hat{K} = \begin{bmatrix} 0 & -t & 0 & 0 \\ -t & 0 & -t & 0 \\ 0 & -t & 0 & -t \\ 0 & 0 & -t & 0 \end{bmatrix}. \tag{1.2}$$

Antiperiodic boundary conditions imply that, upon hopping around the edges, the sign of the hopping constant flips.

3. The molecular one-body counterpart to $\hat{K}$, $\hat{O}$, would consist of all one-body terms connecting an electron of spin σ in a first orbital, i, with an electron of spin σ in a second orbital, j,

$$\hat{O} = \sum_{ij,\sigma} O_{ij,\sigma} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma}, \tag{1.3}$$

where $O_{ij,\sigma}$ denotes the corresponding one-body integrals over orbitals.

1.0.2 Exercise Solutions

1. The non-interacting solution may be obtained by simply diagonalizing the matrix $\hat{K}$, since the non-interacting Hamiltonian is $\hat{H} = \hat{K}$ and solving this Hamiltonian simply requires diagonalizing it. Numpy has convenient linalg routines for diagonalizing matrices.

2. If a wave function represents 2 up electrons and 3 down electrons, it will consist of the outer product of a spin-up determinant containing the first 2 leading non-interacting eigenvectors (the eigenvectors corresponding to the 2 lowest energies) and a spin-down determinant containing the first 3 non-interacting leading eigenvectors. In the general case, a wave function with k up electrons and l down electrons will consist of the outer product of a determinant containing the first k eigenvectors and a determinant containing the first l eigenvectors. (Note that, here, we assume the spin-up and spin-down terms in the non-interacting Hamiltonian are the same.)

3. $\hat{K}$ is an NxN matrix, which is significantly smaller than $\hat{H}$, which scales exponentially with N when expressed in terms of all of the possible states of the system. Whereas the process of diagonalizing $\hat{H}$ therefore scales exponentially, multiplying one-body operators as AFQMC does only scales as N^3.

2 Propagation in AFQMC

2.1 Propagating the Non-Interacting Hamiltonian Wave Function

2.1.1 Exercise Solutions

1. To obtain $e^{-\Delta\tau\hat{K}}$, one must simply exponentiate the matrix $-\Delta\tau\hat{K}$. This can be done using the linalg expm method.

2. See solutions code. One must construct and store this matrix exponential and then repeatedly multiply it into the wave function.

3. To compare your wave function after each propagation step, you should orthonormalize it first (see the orthogonalization routines). You can then use a norm of your choice to compare wave functions to one another. Note that, for the non-interacting case, because you are starting with a non-interacting trial wave function, your wave function should remain the same after each propagation step (propagating the non-interacting trial wave function to obtain the non-interacting solution should not change the wave function because you already started with the exact answer!). Regardless, tracking the energy is a more meaningful way to track convergence (see below).

2.2 *(Advanced)* Measuring the Energy

2.2.1 Exercise Solutions

1. See solution code.

2. To check your non-interacting propagation, check that your printed energy remains the same (-4 in units of t) after every propagation step.

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

3.0.1 Exercise Solutions

1. Your check should be that, after enough sampling, you should obtain $e^{y^2/2}$ within some error.

3.1 The Operator Hubbard-Stratonovich Transformation

3.1.1 Exercise Solutions

1. The key observation is that $n_\uparrow^2 = n_\uparrow$ because $n_\uparrow$ can equal either 0 or 1 for fermions. The same logic applies to $n_\downarrow^2$. As such

$$= -\frac{(\hat{n}_\uparrow - \hat{n}_\downarrow)^2}{2} + \frac{\hat{n}_\uparrow + \hat{n}_\downarrow}{2} \tag{3.1}$$

$$= -\frac{\hat{n}_\uparrow - 2\hat{n}_\uparrow\hat{n}_\downarrow + \hat{n}_\downarrow}{2} + \frac{\hat{n}_\uparrow + \hat{n}_\downarrow}{2} \tag{3.2}$$

$$= \hat{n}_\uparrow\hat{n}_\downarrow. \tag{3.3}$$

2. Once a gaussian-distributed field, x_i, is sampled, to construct the HS-Transformed one-body propagators, two constants should be constructed for the spin-up and spin-down terms. For the spin-up term, $e^{x_i\sqrt{\Delta\tau U}}$ should be constructed, while for spin-down, $e^{-x_i\sqrt{\Delta\tau U}}$ should be constructed. Since these multiply the density, $\hat{n}_i$, to apply

the full operators, multiply row i in the spin-up and spin-down matrices by these respective constants. See the solution code for more details. The $e^{-\Delta\tau U(\hat{n}_{i\uparrow}+\hat{n}_{i\downarrow})/2}$ term from the HS-Transformation is just a constant (it doesn't contain an operator), so it can simply be multiplied into the spin-up and spin-down wave functions.

3. After performing the HS Transformation, the one-body operator from this transformation is $e^{-x_i\sqrt{-\Delta\tau U}\hat{n}_{i\uparrow}}$. If $U > 0$, the operator requires the square root of a negative number, $-\Delta\tau U$. This square root yields a complex number, which causes the phase problem. The phase problem may obviously be avoided by using the optimal transformation in this simple Hubbard case, but is more difficult to avoid when the general Coulomb potential is used.

4. See solutions code.

4 Illustrative AFQMC Simulation

4.1 Implementing the AFQMC Inner Propagation Loop

4.1.1 Exercise Solutions

1. Perform the same matrix exponentiation as before, just divide $\hat{K}$ by 2.

2. See solutions code.

3. In order to evaluate the potential contribution to the total energy, $U\langle\hat{c}^\dagger_{i\uparrow}\hat{c}_{i\uparrow}\hat{c}^\dagger_{i\downarrow}\hat{c}_{i\downarrow}\rangle$, which notably contains a two-body density matrix, must be evaluated. In this case, the two-body density matrix may be reduced to a product of one-body density matrices using Wick's Theorem to yield

$$U\langle\hat{c}^\dagger_{i\uparrow}\hat{c}_{i\uparrow}\hat{c}^\dagger_{i\downarrow}\hat{c}_{i\downarrow}\rangle = U\langle\hat{c}^\dagger_{i\uparrow}\hat{c}_{i\uparrow}\rangle\langle\hat{c}^\dagger_{i\downarrow}\hat{c}_{i\downarrow}\rangle. \tag{4.1}$$

Since you have already evaluated the one-body density matrices, this quantity is now easily evaluated by multiplying the correct diagonal elements of the spin-up and spin-down one-body density matrices.

4.2 Weighting and Walkers

4.2.1 Exercise Solutions

1. See solutions code. As you will be more thoroughly sampling the Hubbard-Stratonovich Transformation, you should see the accuracy of your results increase as the number of walkers is increased. You can check this by obtaining exact diagonalization results for a small representative system, calculating error bars (as discussed during different portions of this school), and watching those error bars decrease in size as the number of walkers increases. Now, without population control, some walkers will tend to either large or small weights. Population control assists with taming large-weighted walkers.

2. Feel free to use any techniques learned during the school. Virtually all of them are valid in this context. Birth/death methods are most common in AFQMC. Russian roulette and comb methods have also been employed.

4.3 Future Thoughts

4.3.1 Exercise Solutions

1. The full, non-relativistic *ab initio* Hamiltonian in second-quantization may be written as

$$\hat{H} = \sum_{ij} T_{ij} \left(\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i \right) + \sum_{ijkl} V_{ijkl} \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_l \hat{c}_k, \tag{4.2}$$

   where i, j, k, and l denote spinorbitals. To perform a Hubbard-Stratonovich Transformation on this, the two-body operators must be transformed into squares of operators, which can be achieved via exact diagonalization or decompositions such as the Cholesky decomposition. Unlike the Hubbard case, those decompositions will typically lead to exponentials of off-diagonal operators, which will make your propagators more complicated and off-diagonal. However, the underlying transformation is the same as you coded.

2. The constrained path approximation ensures that a walker is weighted to zero whenever a determinant's overlap with the initial wave function becomes 0. There are ways of easing a walker to 0 weight to prevent large jumps in weights. The phaseless approximation essentially projects all complex weights to the real axis using a cosine function, after the exponentials, and therefore the complexity, are made as small as possible.

5 References

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