# Quantum-Classical Auxiliary-Field Quantum Monte Carlo

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Auxiliary-Field Quantum Monte Carlo (AFQMC) is a powerful method for solving electronic structure problems, particularly in strongly correlated systems. It uses auxiliary fields to simplify two-body interactions but is limited by the fermionic sign problem as well as its expensive computations of wavefunction overlap. Quantum-Classical AFQMC (QC-AFQMC) integrates quantum computing to accelerate overlap measurements and mitigate the sign problem. This paper explores the theoretical basis of QC-AFQMC and its potential for accurately modeling strongly-correlated systems. Techniques such as shadow tomography are also discussed for improving efficiency.

## I. INTRODUCTION

In 1982, Richard Feynman proposed the use of quantum computers to simulate physical systems, highlighting their potential to model complex quantum phenomena beyond the capabilities of classical computation [1]. The quantum phase estimation (QPE) algorithm, introduced in 1995, was recognized for its ability to calculate ground and excited state energies of molecular systems [2]. However, implementing QPE for meaningful chemical problems requires quantum hardware that is significantly larger and less noisy than current technology, limiting its current applications to small systems [3].

In 2018, John Preskill introduced the concept of the "Noisy Intermediate-Scale Quantum" (NISQ) era - a period in which quantum algorithms must balance resilience to noise with the ability to produce meaningful results on imperfect quantum hardware [4]. Among the early candidates for NISQ algorithms was the variational quantum eigensolver (VQE), proposed in 2014 [5]. VQE employs a hybrid quantum-classical approach to determine molecular ground state energies and is well-suited to existing noisy hardware. However, it faces significant challenges: selecting an appropriate ansatz that enables the classical optimizer to find a global (or near-global) minimum is difficult, and the ansatz must be implementable within the constraints of noisy devices. While small levels of noise can be partially absorbed by the classical optimization step, excessive noise degrades optimization performance as it leads to essentially random outputs when evaluating the Hamiltonian [6].

Recently, the quantum-classical auxiliary-field quantum Monte Carlo (QC-AFQMC) algorithm has emerged as a promising alternative for the NISQ era. This method is particularly effective for strongly correlated systems, such as those encountered in battery chemistry, high-temperature superconductors, and metal-organic frameworks for carbon capture [7]. Unlike VQE, QC-AFQMC does not explicitly represent the ground-state wavefunction on the quantum processor. Instead, it uses auxiliary fields to decouple interactions, allowing for the calculation of ground-state properties without the need for an explicit wavefunction representation [8, 9].

## II. THEORETICAL BACKGROUND

### A. Quantum Monte Carlo

Quantum Monte Carlo (QMC) methods are widely used to simulate many-body quantum systems by stochastically sampling quantum mechanical observables. These methods are especially powerful for strongly correlated systems where mean-field approaches fail [7].

In QMC, the ground-state wavefunction $|\Psi_0\rangle$ of a many-body Hamiltonian $\hat{H}$ can be projected from a trial state $|\Psi_T\rangle$ via imaginary time propagation, following

$$|\Psi_0\rangle \propto \lim_{\tau\to\infty} e^{-\tau\hat{H}} |\Psi_T\rangle \tag{1}$$

where $\tau = it$ and $\langle\Psi_0|\Psi_T\rangle = 0$. Numerically, this limit can be obtained by iterating over the timestep $\Delta\tau$:

$$|\Psi^{(n+1)}\rangle = e^{-\Delta\tau\hat{H}} |\Psi^{(n)}\rangle \tag{2}$$

in which $|\Psi^{(0)}\rangle = |\Psi_T\rangle$, that is, the trial wavefunction is the wavefunction of our first step. QMC methods carry out this iterative process via Monte Carlo sampling.

The ground state energy can then be obtained via the expectation value of the Hamiltonian:

$$E_0 = \lim_{n\to\infty} \frac{\langle\Psi_T|\hat{H}|\Psi^{(n)}\rangle}{\langle\Psi_T|\Psi^{(n)}\rangle} \tag{3}$$

In this situation, we have a mixed estimator that is exact [8]. As the imaginary time $\tau$ increases, the wavefunction $|\Psi_T\rangle$ approaches the ground state $|\Psi_0\rangle$, and the energy estimate of $E_0$ converges to the ground state energy.

### B. Auxiliary-Field Quantum Monte Carlo

AFQMC is a Quantum Monte Carlo technique that utilizes random walks alongside an auxiliary field to simulate the imaginary-time evolution of a quantum system, ultimately converging to its ground state. AFQMC

methods work in the second quantized representation of the Hamiltonian and the auxiliary field space to represent the wavefunction and carry out the integration [8, 10]. In the second quantization, the electronic Hamiltonian is

$$\hat{H} = \hat{H}_1 + \hat{H}_2 = \sum_{pq} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{pqrs} v_{pqrs} a_p^\dagger a_q^\dagger a_s a_r \quad (4)$$

where $a_p^\dagger$ and $a_q$ are the creation and annihilation operators of orbitals $p$ and $q$, respectively. The term $h_{pq}$ represents the matrix elements of the one-body Hamiltonian interactions, $\hat{H}_1$, and the term $v_{pqrs}$ is the matrix elements of the two-body ($\hat{H}_2$) interactions of $\hat{H}$.

For a small but non-zero $\Delta\tau$, the Trotter approximation may be used for the iterative time propagation in Eq. (2)

$$e^{-\Delta\tau\hat{H}} \approx e^{-\Delta\tau\hat{H}_1} e^{-\Delta\tau\hat{H}_2} \quad (5)$$

This approximation introduces Trotter error; to minimize this error, generally higher-order Trotterization is used in a real implementation of this algorithm.

The $\hat{H}_1$ term in Eq. (5) is a one-body operator, while the $\hat{H}_2$ term is not and must be rewritten in this form using a Hubbard-Stratonovich (HS) transformation. Different HS transformations exist and can impact the accuracy of the QMC algorithm. By introducing the collection of auxiliary fields $\mathbf{x}$, the following outcome of one form of the HS transformation is

$$e^{-\Delta\tau\hat{H}} = \int d\mathbf{x}\; p(\mathbf{x})\; \hat{B}(\mathbf{x}) \quad (6)$$

where $p(\mathbf{x})$ is a probability distribution function, and $\hat{B}(\mathbf{x})$ is a one-body propagator obtained from the one-body operators coupled to $\mathbf{x}$. Specifically, $\hat{B}$ is defined by the following equation

$$\hat{B} = e^{\sum_{ij} c_i^\dagger U_{ij} c_j} \quad (7)$$

Where $U$ is a square matrix whose elements are given by $U_{ij}$ and $B \equiv e^U$.

The Hubbard–Stratonovich (HS) transformation reformulates two-body interactions as one-body interactions influenced by stochastic auxiliary fields. Effectively, this approach maps an interacting quantum system onto a collection of non-interacting systems, each subject to dynamic, fluctuating auxiliary fields. By summing over all possible auxiliary field configurations, the original two-body interactions are reconstructed.

### C. The Sign Problem

The sign problem arises from the antisymmetric nature of the fermionic wavefunction. In QMC, sampling weights can become negative or complex due to interference effects, leading to poor statistical convergence.

A common solution to this problem is to create a modified update rule which constrains the path of the walkers. This introduces a bias which affects the accuracy of the results, the magnitude of which depends largely on the quality of the initial trial state.

### D. Monte Carlo Sampling via a Random Walk

$|\Psi_T\rangle$ can be initialized to the Hartree-Fock solution $|\Psi_{HF}\rangle$. The initial wavefunction can be thought of as a sum of Slater determinants, called "walkers" for this algorithm:

$$|\Psi_T\rangle = \sum_k w_k^{(0)} |\psi_k^{(0)}\rangle \quad (8)$$

where $k$ is the number of walkers, and $w_k^{(0)} = 1$ and $|\Psi_k^{(0)}\rangle = |\Psi_{HF}\rangle$. When the projection is applied to this initial state as in Eq. (3), the wavefunction after $n$ steps is represented as

$$|\Psi^{(n)}\rangle = \sum_k w_k^{(n)} |\psi_k^{(n)}\rangle \quad (9)$$

The projection to each new step goes like Eq. (1). Using Eq. (6), we can sample our probability distribution function $p(\mathbf{x})$ to obtain the auxiliary field $\mathbf{x_k}$.

$$|\Psi^{(n+1)}\rangle = \hat{B}(\mathbf{x_k}) |\psi_k^{(n)}\rangle \quad (10)$$

Throughout the random walk, the Gram-Schmidt procedure is applied to each walker, and a renormalization factor is included in each $w_k^{(n+1)}$. As some walkers will gradually contribute more than others, a population control measure must be implemented to replicate the walkers with larger weights and eliminate the ones with smaller weights [7].

## III. QUANTUM-CLASSICAL AUXILIARY-FIELD QUANTUM MONTE CARLO

QC-AFQMC integrates quantum computing into the AFQMC framework to enhance its accuracy and scalability. Quantum computers could address key bottlenecks in the classical algorithm, particularly in preparing trial wavefunctions and evaluating overlaps [9]. Quantum-prepared trial states, such as those generated using methods like the Unitary Coupled Cluster (UCC) ansatz, can achieve higher overlap with the ground state, thereby mitigating errors introduced by solutions to the sign problem. The unitary coupled cluster (UCC) ansatz,

widely used in variational quantum algorithms, is particularly advantageous because it intrinsically captures electron correlations, improving the accuracy of AFQMC simulations and reducing the impact of pathological configurations [11].

A key consideration to implementing QC-AFQMC is to determine how to evaluate the overlap amplitude $\langle\Psi_t|\psi_k^{(0)}\rangle$ for each walker. As there is currently significant overhead and latency in resetting and initialization of quantum circuits, as well as communication between quantum and classical processors, the large number of walkers in a typical AFQMC implementation can be a problem in some implementations of this overlap measurement. However, shadow tomography has proven to be a useful technique to measure these overlaps while avoiding these bottlenecks.

### A. Implementation with Classical Shadows

The protocol for measuring wavefunction overlap with classical shadows is as follows. Let $\rho$ be the density matrix of an n-qubit quantum state, and $\{O_i\}$ be a collection of observables for which we will estimate the expectation values, $tr(O_i\rho)$. With classical shadow tomography, this estimate has only a logarithmic computational cost using the following procedure:

1. Choose a set of unitary transformations, $\mathcal{D}$
2. Sample random unitaries $U \in \mathcal{D}$
3. Measure the state $U\rho U^\dagger$ in the basis $|b\rangle$ to obtain $|b\rangle\langle b|$

Our quantum channel $\mathcal{M}$ is then defined by:

$$\mathcal{M}(\rho) \coloneqq \mathbb{E}[U^\dagger |\hat{b}\rangle \langle\hat{b}| U] \tag{11}$$

where $\mathbb{E}$ denotes averaging, and the hat a statistical estimator.

As long as measuring in the basis is tomographically complete, we may apply $\mathcal{M}^{-1}$ to Eq. (11) to obtain

$$\rho = \mathbb{E}[\mathcal{M}^{-1}(U^\dagger |\hat{b}\rangle \langle\hat{b}| U)] \tag{12}$$

The collection $\{\mathcal{M}^{-1}(U^\dagger |\hat{b}\rangle \langle\hat{b}| U)\}$ is called the classical shadows of $\rho$.

We can use these shadows to estimate the expectation values $tr(O_i\rho)$ via

$$\langle O_i\rangle = \mathbb{E}\ tr[O_i\mathcal{M}^{-1}(U^\dagger |\hat{b}\rangle \langle\hat{b}| U)] \tag{13}$$

to within an error $\epsilon$ [11, 12].

In this implementation, it is desirable that there exist an efficient method to sample $U$ from $\mathcal{D}$, and to compute the expectation values with respect to the shadows on a classical computer.

Several groups have explored using Matchgate shadows and found it advantageous over Clifford shadows by eliminating the need for an exponentially scaling post-processing step [11, 13]. Furthermore, implementation with Matchgate shadows has been proven to be robust to noise [11]. Despite this, the overall post-processing costs for QC-AFQMC are still high, and implementation of this algorithm for chemically relevant systems (e.g., FeMoCo) would require significant classical parallelization and/or further optimizations to the algorithm.

## IV. QUANTUM ADVANTAGE DISCUSSION

One argument in favor of quantum advantage is that with matchgate shadows, the variance scales with system size like $\mathcal{O}(\sqrt{N}logN)$, requiring the measurement of only a polynomial number of samples - better than the computational complexity of the classical algorithm for calculating overlap, which scales as $\mathcal{O}(N^4)$ [13].

However, for the whole algorithm including all post-processing steps, a computational advantage in speed is yet to be seen. Thus, the stronger argument for potential quantum advantage in the QC-AFQMC algorithm is the improved accuracy of the solution due to the fact that beginning with a trial wavefunction closer to the ground state (such as UCC) aids in unbiasing the walker paths in the phaseless, constrained version of the problem.

A major remaining issue with the algorithm is that as system size increases, the overlap integrals $\langle\Psi_T|\psi_k^{(0)}\rangle$ decay at an exponential rate. This necessitates an exponentially increasing number of shots in order to reduce the relative errors of the overlap to within an acceptable level. This issue exists for both the classical and quantum QMC methods. Ref. [11] suggests that if this issue can be mitigated, then practical quantum advantage could be achieved for system sizes comprising roughly 100 orbitals.

## V. CONCLUSION

Quantum-Classical Auxiliary-Field Quantum Monte Carlo (QC-AFQMC) combines quantum computing with classical AFQMC to tackle the ground state problem for strongly correlated electronic systems. By improving trial wavefunctions and overlap measurements, it has the potential to provide more accurate energies than its classical counterpart. Moreover, its high resilience to noise makes it especially attractive in the NISQ era. While challenges remain, such as mitigating the exponential decay of overlaps as well as optimizing classical post-processing, QC-AFQMC represents a promising step toward practical quantum applications in electronic structure problems. As quantum technologies mature, QC-AFQMC could redefine how we approach complex quantum systems in the NISQ era and beyond.

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