Simulating the Mott transition on a noisy digital quantum computer via Cartan-based fast-forwarding circuits

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Dynamical mean-field theory (DMFT) maps the local Green’s function of the Hubbard model to that of the Anderson impurity model and thus gives an approximate solution of the Hubbard model by solving the simpler quantum impurity model. Quantum and hybrid quantum-classical algorithms have been proposed to efficiently solve impurity models by preparing and evolving the ground state under the impurity Hamiltonian on a quantum computer instead of using intractable classical algorithms. We propose a highly optimized fast-forwarding quantum circuit to significantly improve quantum algorithms for the minimal DMFT problem preserving the Mott phase transition. Our Cartan decomposition based algorithm uses a fixed depth quantum circuit to eliminate time-discretization errors and evolve the initial state over arbitrary times. Exploiting the structure of the fast-forwarding circuits, we sufficiently reduce the gate cost to simulate the dynamics of, and extract frequencies from, the Anderson impurity model on noisy quantum hardware and demonstrate the Mott transition by mapping the phase-diagram of the corresponding impurity problem. Especially near the Mott phase transition when the quasiparticle resonance frequency converges to zero and evolving the system over long-time scales is necessary, our method maintains accuracy where Trotter error would otherwise dominate. This work presents the first computation of the Mott phase transition using noisy digital quantum hardware, made viable by a highly optimized computation in terms of gate depth, simulation error, and run-time on quantum hardware. The combination of algebraic circuit decompositions and model specific error mitigation techniques used may have applications extending beyond our use case to solving correlated electronic phenomena on noisy quantum computers.

I. INTRODUCTION

Using quantum computers to accurately model the behavior of strongly correlated quantum systems is one of the most promising near-term applications of noisy intermediate scale quantum (NISQ) computers. For example, quantum simulations of fermions only require ~100 qubits to potentially surpass classical simulation methods. In contrast, Shor’s algorithm [1] for factoring large numbers will require thousands of nearly-noiseless qubits to become practically useful. Proposals for simulating correlated fermionic systems using quantum computers exist [2–7] but relatively few have been implemented or tested due to the noise of current devices [8–10].

Within condensed-matter physics a wide variety of correlated systems can be mapped to correlated impurity models by embedding methods such as dynamical mean-field theory (DMFT). Even though the DMFT impurity mapping simplifies many problems, classical simulations based on exact diagonalization are still limited to dozens of orbitals [11] due to the exponential growth of correlations and the corresponding Hilbert space which requires an exponential amount of memory to store the quantum many-body state. Other methods, such as quantum Monte Carlo (QMC) [12] and matrix product state (MPS) [13] methods, also suffer from some sort of exponential complexity scaling making them intractable. In the case of QMC, the fermion sign problem [14] has been shown to be NP-hard in general and limits simulations to high temperatures. Matrix product state methods, on the other hand, suffer from entanglement issues for certain geometries [13]. Quantum computers alleviate this exponential scaling by instead storing many-body quantum states with memory resources scaling polynomially with the system size.

Prior work studying the dynamics of interacting electrons via DMFT observed that even over very small time scales Trotter approximate time evolutions lead to nonphysical results: comparing to theoretical values, simulations on the quantum computer give inaccurate frequencies of the time evolution for the two-site DMFT, which are symptoms of decoherence or approximation errors [10]. For NISQ systems, the Trotter approximation leads to a dilemma: theoretically it becomes exact in the limit of an infinite-depth circuit, so more accurate simulations require increased gate counts, but increasing gate count reduces simulation fidelity due to accumulated noise. The hardware requirements...
needed to achieve reliable updates in the DMFT loop using the Trotter decomposition of the time evolution operator has been analyzed in Ref. 15. In Ref. 9, the authors use a variational quantum eigensolver (VQE) to implement an exact diagonalization solver for the two-site DMFT problem. This method works well for two-site DMFT after a regularization technique is used to remove the unphysical pole that arises from small errors, but the usefulness of the method depends on the scalability of VQE.

In this work, we approach solving the two-site DMFT problem by utilizing a Lie-algebraic method to fast-forward the dynamics of the Anderson Impurity Model (AIM). Our method, based on a Cartan decomposition of the algebraic closure of the Hamiltonian, compiles the time evolution operator into a fixed depth circuit for any chosen simulation time; therefore, the error from the quantum device is independent of the length of the time evolution of the system and a one-time decomposition performed on a classical computer allows for arbitrarily low numerical error in the parameters of the decomposed factors. As described in Ref. 16, given a Hamiltonian \( \hat{H} \), the Cartan decomposition requires finding a particular sequence of unitary rotations which, when contracted, span and parameterize the time evolution unitary \( e^{-itH} \) of a target system for all time \( t \). The Cartan decomposition generalizes the polar and singular-value decompositions at the level of groups and provides a mapping from the required dynamics onto two sets of parameterized unitaries.

We first review and motivate the quantum impurity model and provide a hybrid quantum-classical algorithm solving it. We then apply group analysis to fast-forward the dynamical simulation on a quantum computer. The structure of Cartan decomposition allows for further simplifications which result in a highly optimized circuit that can be tailored to execute on specific hardware architectures. We then perform simulations at vastly different time scales which allow us to accurately extract both low and high frequency Green’s functions for the two-site DMFT on NISQ hardware. This enables us to demonstrate for the first time a Mott-insulating phase transition in the Hubbard model via a digital quantum simulation on quantum hardware.

## II. MODEL HAMILTONIANS

### A. Hubbard model

The Fermi-Hubbard (referred as Hubbard below) model has no known exact solution in more than one dimension, even though its Hamiltonian has a simple form where the interactions between fermionic particles (i.e., Coulomb interactions between electrons) are reduced to a constant on-site interaction \( U \geq 0 \). Despite this deceptive simplicity, the Hubbard model can account for many interesting quantum phenomena in condensed matter physics, including the Mott metal-insulator transition [17–19], antiferromagnetism [20], emergent spin and stripe orders [21, 22], strange metallic behavior [23], pseudogaps [24, 25], and high-temperature superconductivity [24, 26].

The single-band Hubbard model Hamiltonian is given by

\[
\hat{H}_{\text{Hub}} = -t \sum_{\langle i,j \rangle, \sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \hat{c}_{j\sigma}^\dagger \hat{c}_{i\sigma}) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \mu \sum_i \hat{n}_{i,\sigma},
\]

where \( \hat{c}_{i\sigma}^\dagger (\hat{c}_{i\sigma}) \) is the electron creation (annihilation) operator for electron with spin \( \sigma \in \{\uparrow, \downarrow\} \) at lattice site \( i \), \( \hat{n}_{i\sigma} = \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma} \) is the electron density operator, \( t \) is the hopping integral (“tunneling”), \( U \) is the on-site Coulomb interaction, and \( \mu \) is the chemical potential. Here, \( \langle i, j \rangle \) refers to indices of nearest-neighbor sites \( i \) and \( j \) [27]. The Hubbard model has been recently investigated in the context of quantum computing with the applications of VQE algorithms [28, 29] and as a benchmark for quantum simulations [4, 30, 31].

### B. Anderson impurity model and dynamical mean-field theory

Simulations of the Hubbard model are limited to dozens of fermionic orbitals [32–34], far from the large number of particles which would be considered in the macroscopic (thermodynamic) limit. Dynamical mean-field theory is a significant development in studying the Hubbard model for larger systems [35]. In the limit of a lattice with infinite dimensions (\( \infty-d \)), such as \( \infty-d \) hypercubic Bethe lattice with infinite coordination number, DMFT exactly maps the solution of the Hubbard model to that of the Anderson impurity model, where the temporal correlations are accurately captured. The interacting electrons in the Hubbard model in the thermodynamic limit (i.e., \( \infty \) lattice sites) are reduced to electrons interacting on a single impurity site coupled to an electronic bath of continuous levels that tunnel into the impurity site. We describe the energy levels using \( N_b \) discrete bath lattice sites with on-site energy \( \epsilon_i \) and index \( i \in \{1, \ldots, N_b\} \). When the number of bath sites is infinite, the DMFT solution will exactly match the solution

- \( \epsilon \in \{ \uparrow, \downarrow \} \)
- \( \epsilon \in \{ i \} \)
- \( \epsilon \in \{ 1 \}
- \( \epsilon \in \{ \} \)
- \( \epsilon \in \{ 0 \} \)
of the original Hubbard model. Since we will consider nonmagnetic states, these parameters do not depend on the electron spin quantum number \( \sigma \). The Anderson impurity model Hamiltonian is then given by

\[
\hat{H}_{\text{AIM}} = \sum_{i=1,\sigma}^N V_i (\hat{c}_{i,\sigma}^\dagger \hat{c}_{i,\sigma} + \hat{c}_{i,\sigma} \hat{c}_{i,\sigma}^\dagger) + U \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} + \sum_{i=0,\sigma}^N (\epsilon_i - \mu) \hat{n}_{i,\sigma},
\]

where hybridization parameter \( V_i \) is the hopping between the impurity site (site-index \( i = 0 \)) and bath sites (site-index \( 1 \leq i \leq N_b \)). The Coulomb interaction \( U \)-term only involves the impurity site.

The minimal nontrivial approximation of the Hubbard model dynamics is two-site DMFT \([36]\), involving the impurity site and only one bath site \((N_b = 1)\). This is the case we will consider. As shown in appendix A, after the Jordan-Wigner fermion-spin transformation, equation (2) in fermion operators becomes the impurity Hamiltonian in Pauli string operators given by

\[
\hat{H}_{\text{AIM}} = \frac{V}{2}(X_0 X_1 + Y_0 Y_1 + X_2 X_3 + Y_2 Y_3) + \frac{U}{4} Z_0 Z_2.
\]

Here, \( X_l, Y_l, Z_l \) are single-qubit Pauli string operator on qubit index \( l \). Specifically, the spin-up (spin-down) modes on the impurity site 0 and the bath site 1 are mapped to qubit index 0 and 1, respectively (qubit index 2 and 3, respectively). In addition, we only consider the half-filled paramagnetic ground state, so the impurity Hamiltonian equation (3) has been simplified by setting \( \mu = \frac{U}{2}, \epsilon_0 = 0, \) and \( \epsilon_1 = \frac{U}{2} \) in equation (2).

### III. ALGORITHM AND METHODS

#### A. Algorithm for computing Green’s function

In DMFT, the dynamic response of the interacting electron system is described by the *retarded impurity Green’s function* denoted as \( G^{R,\uparrow}_{\text{imp}}(t, t') \) (for spin-up orbital on the impurity site) in the time domain and is given by

\[
G^{R,\uparrow}_{\text{imp}}(t, t') = -i\theta(t - t') \langle \psi_0 | \{ \hat{c}_0(t), \hat{c}_0^\dagger(t') \} | \psi_0 \rangle,
\]

where \( \theta(t) \) is the step-function, \( \hat{c}_0(t) = U^\dagger(t) \hat{c}_0 U(t), \hat{c}_0^\dagger(t) = U^\dagger(t) \hat{c}_0^\dagger U(t) \), time evolution operator \( U(t) = e^{-it\hat{H}_{\text{AIM}}} \), and \( | \psi_0 \rangle \) is the many-body ground state of the impurity Hamiltonian \( \hat{H}_{\text{AIM}} \) (the subscript "0" in \( | \psi_0 \rangle \) indicates ground state, not site index 0). Due to time-translation invariance of a time-independent Hamiltonian \( \hat{H}_{\text{AIM}} \), we simplify the computation by setting \( t' = 0 \). We only consider the paramagnetic ground state, the impurity Green’s function is diagonal in spin-space \( G^{R,\sigma\sigma'}_{\text{imp}}(t) = G^{R,\sigma}_{\text{imp}}(t) \delta_{\sigma\sigma'} \) and \( G^{R,\uparrow}_{\text{imp}}(t) = G^{\text{imp}}_{\text{imp}}(t) \). We therefore drop the spin index in the remainder of this work and denote the impurity Green’s function by \( G^{R}_{\text{imp}}(t) \).

In appendix B we elaborate on the full expansion and subsequent simplification of Green’s function after the Jordan-Wigner transform is applied, which results in the relatively inexpensive expectation

\[
i G^{R}_{\text{imp}}(t > 0) = \text{Re} \langle \psi_0 | U^\dagger(t) X_0 U(t) X_0 | \psi_0 \rangle.
\]

This term can be measured with a single Hadamard-test type quantum circuit using only a single time evolution unitary as discussed later (see figure 3 panels b,c).

#### 1. Iteration loop for DMFT

The DMFT mapping is a self-consistent mapping, requiring multiple iterations where the DMFT parameters \( V_i \) and \( \epsilon_i \) are updated, from an initial guess of the Anderson impurity model, until the system reaches self-consistency. For each new iteration, the \( V_i \) and \( \epsilon_i \) computed in the previous iteration are put back into the impurity model, which is then solved and the solution used to recompute the DMFT parameters. The iteration loop continues until the recomputed values are sufficiently close to the previous values of \( V_i \) and \( \epsilon_i \). For the two-site model, particle-hole symmetry and the structure of the two-site solution provide a mechanism for reducing the cost of the computation.
Given $U$, initialize parameter $V$

**DMFT Loop**

- Compute Cartan parameters $\{\vec{h}, \vec{k}_0, \vec{k}_1\}$
- Update impurity model $H_{\text{AIM}}$  
- V (or $Z$) value self-consistent?
- Yes
- Update $V = \sqrt{Z}$
- No

- Simulate $G(t_{\text{high}})$
- Extract $\omega_2$ from DFT of $G(t_{\text{high}})$
- Valid $\omega_2$?
- No
- Compute $Z = [1 - \text{dRe} \Sigma(\omega)/\text{d} \omega]^{-1}$
- Yes

- Simulate $G(t_{\text{low}})$
- Extract $\omega_1$ from DFT of $G(t_{\text{low}})$
- Valid $\omega_1$?
- No

**Hybrid $\Sigma(\omega)$ calculation**

FIG. 1: Diagram of the DMFT loop specialized for the two-site calculation. Our calculations are initialized with $V = 0.5$. Each DMFT loop iteration also updates the time evolution Cartan parameters corresponding to the updated $V$. The hybrid computation of $\Sigma(\omega)$ evaluates the two frequencies $\omega_1$ and $\omega_2$ separately, in a procedure that is elaborated on in section IV(C).

and the accuracy of convergence.

The form of the DMFT loop used for our calculations can be summarized as follows and is represented in figure 1:

1. Choose initial values for parameters $V_i$ and $\epsilon_i$. Due to half-filling of the two-site model, the values for $\epsilon_0$ and $\epsilon_1$ are fixed and do not need to be updated.

2. On the quantum computer, evaluate the retarded impurity Green’s function $G_{\text{imp}}^R(t)$ for a selection of time $t$ values. In the two-site model, the evaluated function will have the form

$$iG_{\text{imp}}^R(t > 0) = 2[\alpha_1 \cos(\omega_1 t) + \alpha_2 \cos(\omega_2 t)]$$

where $\omega_1$ is the quasi-particle resonance frequency and $\omega_2$ is the Hubbard band [36].

3. Compute the discrete Fourier transform (DFT) of Green’s function, giving $G_{\text{imp}}^R(\omega)$.

4. Compute the self-energy $\Sigma_{\text{imp}}(\omega)$ using $G_{\text{imp}}^R(\omega)$. We have the general result [37]

$$G_{\text{imp}}^R(\omega) = \frac{1}{\omega + i\delta - (\epsilon_0 - \mu) - \Delta(\omega) - \Sigma_{\text{imp}}(\omega)}.$$  

which introduces an artificial broadening term $i\delta$. $\Delta(\omega)$ is the mean-field-like hybridization function

$$\Delta(\omega) = \frac{V^2}{\omega - (\epsilon_1 - \mu) + i\delta}.$$  

Dyson’s equation $G_{\text{imp}}^R(\omega) = G_{\text{imp}}^R(0) + G_{\text{imp}}^R(0)\Sigma_{\text{imp}}(\omega)G_{\text{imp}}^R(\omega)$, along with the result in equation (7) provides an analytic solution

$$\Sigma_{\text{imp}}(\omega) = \frac{1}{G_{\text{imp}}^R(0)} - \frac{1}{G_{\text{imp}}^R(\omega)},$$
Here, $G_{imp}^{(0)}(\omega)$ is the non-interacting Green’s function with $U = 0$. In the frequency domain, this is exactly

$$G_{imp}^{R(0)}(\omega) = \frac{1}{\omega - \left(\epsilon_0^{(0)} - \mu^{(0)}\right) - \Delta(\omega)} = \frac{1}{\omega - \Delta(\omega)}. \tag{10}$$

5. From the self-energy, compute the quasi-particle weight $Z$ and update $V_{\text{new}} = \sqrt{Z}$. In this work, we use the value of the quasi-particle weight computed using the derivative of the self-energy at zero frequency:

$$Z^{-1} = 1 - \left. \text{dRe}[\Sigma_{\text{imp}}(\omega)] \right|_{\omega=0} \text{d} \omega \tag{11}$$

Prior work on this topic by Keen et al. [10] computed the quasi-particle weight as the integral of the spectral function $A(\omega) = -\frac{1}{\pi}\text{Im}[G_{\text{imp}}^{R}(\omega)]$ over the low frequency peaks

$$Z = \int_{|\omega|<4\delta} A(\omega) \text{d} \omega, \tag{12}$$

in order to mitigate noise sources. We initially observed a numerical instability in computing $Z$ using equation (11) which arises from taking the derivative of the self-energy computed using $G_{\text{imp}}^{R}(t)$ fitted to equation (6) without analytically exact solutions for the parameters. Instead of computing the derivative in equation (11) numerically, we solve the derivative analytically in Appendix C by using the exact Fourier integral transform of equation (6), remove the unphysical simple pole of self-energy by assuming a condition obeyed by the exact solution $\frac{\omega_1}{\omega_1^2} + \frac{\omega_2}{\omega_2^2} = \frac{1}{V^2}$, and finally find equation (13), which is equivalent to equation (14) that depends only on the parameters $\omega_1$ and $\omega_2$. In converting equation (13) to equation (14), we use the spectral function sum rule $2\alpha_1 + 2\alpha_2 = 1$.

$$Z = \frac{2(\alpha_1 \omega_2^2 + \alpha_2 \omega_1^2)^2}{\alpha_1 \omega_2^2 + \alpha_2 \omega_1^2} \tag{13}$$

$$= \frac{\omega_1^2 \omega_2^2}{V^2(\omega_1^2 + \omega_2^2 - V^2)}. \tag{14}$$

2. Cartan decomposition

Our primary contribution is simplifying the time evolution unitary operation $\exp\left(-it\hat{H}_{\text{AIM}}\right)$ in the Green’s function measurement circuit by applying Cartan decomposition. The standard method based on Trotterization is an approximation of the time evolution circuit which converges in the limit of an infinite depth circuit. Though there are different methods of approaching a Trotter time evolution, the first order approximation is typically applied [10, 15, 37]:

$$e^{-it\hat{H}} = \left(e^{-i\frac{t}{M}\hat{H}}\right)^N \approx \left(\prod_{l=1}^{M} e^{-i\frac{\beta_l}{M}b_l}\right)^N \tag{15}$$

where $\hat{H} = \sum_{l=1}^{M} \beta_l b_l$ with $\beta_l \in \mathbb{R}$ and $b_l$ is a Pauli string.

The fast-forwarding algorithm used in our time evolution operator is based on the application of an algorithm for performing Cartan decomposition. Here, we briefly summarize the algorithm applied to $\hat{H}_{\text{AIM}}$ given in equation (3) and also illustrate the steps in figure 2. We denote a (real) Lie algebra and its elements by lowercase Gothic (Fraktur) and Roman characters, respectively, such as $g$ and $ig \in g$, where $g$ is a simple $n$-qubit Pauli string or a linear combination of them (with real coefficients). Here, we use the physicists’ convention with a pre-factor $i$ in the Lie algebra elements. $SU(2^n)$ group elements are denoted by uppercase Roman characters, e.g., $G = \exp(i\gamma)$. The goal is to find a factorization of the unitary operator by use of the KHK theorem, which states that the unitary may be written as

$$e^{-it\hat{H}} = e^{i\hat{k}}e^{-ith}e^{-ik} \tag{16}$$

where $k$ and $h$ are elements of a Cartan decomposition (see below). Note that the time argument $t$ only appears in
one factor. The general steps to obtain the Cartan form of the time evolution operator are detailed in Refs. 16 and 38; we briefly summarize them here for completeness.

1. Generate the Hamiltonian algebra \( g(\hat{H}) \). This is a Lie algebra over the field \( \mathbb{R} \) that is generated by the closure of commutators (Lie brackets) of \( ib_i \), where \( b_i \)'s are individual \( n \)-qubit Pauli string terms of the Hamiltonian \( \hat{H} = \sum_i c_i b_i \), \( (c_i \in \mathbb{R}) \). \( g(\hat{H}) \) a subalgebra of \( su(2^n) \).

2. Find a Cartan decomposition \( g = \mathfrak{t} \oplus m \) of the Hamiltonian algebra \( g(\hat{H}) \) such that \( i\hat{H} \) lies in \( m \). Here, \( \mathfrak{t} \) is a subalgebra of \( g(\hat{H}) \).

3. From \( m \) find a largest commuting subalgebra (i.e. a maximal Abelian subalgebra) \( \mathfrak{h} \), which is called a Cartan subalgebra of the pair \( (g, \mathfrak{t}) \).

4. Find a local extremum over the algebra \( \mathfrak{t} \) of \( f(k) = \langle e^{ik}(v) e^{-ik}, \hat{H} \rangle \). Here, \( (a, b) \) is the Killing form which is proportional to \( \text{Tr}(ab) \) for \( a, b \in \mathfrak{su}(2^n) \). \( ik \) is an element of \( \mathfrak{t} \) written as a sum of Pauli strings \( k = \sum_j k_j \) where \( k_j \) form a basis for \( \mathfrak{t} \). The optimization is performed over the coefficients \( \kappa_j \). \( v \) is a fixed element in \( \mathfrak{h} \): \( v = \sum_j \gamma_j^j h_j \) where \( ih_j \) are Pauli strings that form a basis for \( \mathfrak{h} \), and \( \gamma \) is a transcendental number such as \( \pi \). Here, \( \gamma^j \) is the \( j \)-th power of \( \gamma \).

5. Compute the vector \( e^{-ik}(i\hat{H})e^{ik} = ih \). The results of the algorithm are the elements \( ih \in \mathfrak{h} \) and \( ik \in \mathfrak{t} \) which satisfy \( e^{-it\hat{H}} = e^{ik} e^{-it h} e^{-ik} \). Often, additional decomposition is required to implement \( e^{ik} \) using a universal gate set, but in the case of two-site DMFT \( \mathfrak{t} \) is Abelian. Because \( h \) is always composed of commuting elements, the full exponential is relatively simple to implement exactly on a quantum computer. We note that the dimensionality of the Hamiltonian algebra generated by \( \hat{H}_{\text{AIM}} \) scales exponentially with the number of bath sites. However, for the two-site model, the size of the algebra remains manageable. It is of continuing interest to determine if the dimensionality of the Hamiltonian algebra can be constrained to polynomial in the number of bath sites by adopting some effective approximate algorithm.

Analysis of the terms in \( \mathfrak{t} \) resulting from the Cartan decomposition in figure 2(c) reveals that we can divide \( \mathfrak{t} \) into a set of basis elements which commute with \( X_0 \), which we call \( \mathfrak{t}_0 \), and the elements which do not, which we call \( \mathfrak{t}_1 \).

6. Decompose \( \mathfrak{t} \) into \( \mathfrak{t}_0 \) and \( \mathfrak{t}_1 \) such that \( \mathfrak{t} = \mathfrak{t}_0 \oplus \mathfrak{t}_1 \) and \( [\mathfrak{t}_0, X_0] = 0 \).

This step later leads to a reduction in the circuit construction, but we highlight the partition here as an operation which is only possible due to the specific form of the Cartan decomposed time evolution operator.

FIG. 2: (a) A generalized diagram of the Cartan decomposition of the Hamiltonian algebra with dimension = 24 within the special unitary algebra with dimension = 255. Here, \( \mathfrak{t}_0 \) is the set of basis elements which commute with \( X_0 \), which is not a typical requirement of Cartan decomposition but results in a significant gate cost reduction in our application. (b) A block circuit diagram of the decomposed time evolution operator. (c) Cartan decomposition applied to the AIM Hamiltonian equation (A2), where the blue, shaded light blue, magenta, and shaded orange color regions correspond to the sets \( \mathfrak{t}, \mathfrak{t}_0, m, \) and \( \mathfrak{h} \).
Thus instead of preparing as the initial state $\ket{\psi_0}$, we prepare $e^{-ik_0}\ket{\psi_0}$ and time evolve using $e^{ik_1}e^{-ith}e^{-ik_1}$. A combination of manual and algorithmic transpiling through Qiskit reduces the full cost of the final circuit to 77 nearest neighbor CNOTs [41].
Beyond the noise reductions gained through careful compiling of the circuit, we implement three methods in an effort to mitigate errors during the runtime. First, randomized Cartan solutions are employed in an effort to mitigate circuit evaluations are discarded due to this correction, which is applied after all other error mitigation techniques.

Indeed, the final state of the wavefunction qubits is a superposition of two fermions with a total spin zero, so for each shot in the evaluation of Green’s function, we evaluate if the final

of these qubits, instead assuming that the wavefunction qubits are traced out of the final circuit before measuring on the system, or wavefunction, qubits. The Hadamard-test type circuit does not use or require a measurement

The second method to reduce error, measurement error mitigation, serves as an initial step in correcting noise in the experiment results and we process the quantum measurements through the native procedure in Qiskit [41, 43].

The final, and most significant error mitigation technique, follows from post-selection of data from measurements on the system, or wavefunction, qubits. The Hadamard-test type circuit does not use or require a measurement of these qubits, instead assuming that the wavefunction qubits are traced out of the final circuit before measuring $\langle Z_0 \rangle$. The partial trace operation is equivalent to simply measuring the resulting wavefunction state in the $Z$ basis. Indeed, the final state of the wavefunction qubits is a superposition of $|\psi_0\rangle$ and $X_0(t)X_0 |\psi_0\rangle$, both of which we expect to have the same particle number and total spin as the original state $|\psi_0\rangle$. The initial state is known to have two fermions with a total spin zero, so for each shot in the evaluation of Green’s function, we evaluate if the final measurement of the wavefunction state maintains both parameters, discarding the shot if either condition is violated. This corresponds to checking for an odd number of bit-flip errors in the wavefunction qubits which we expect to affect the final ancilla measurement. On the quantum hardware used in this work, $ibmq\_manila$, approximately 65% of the circuit evaluations are discarded due to this correction, which is applied after all other error mitigation techniques.
FIG. 5: DMFT step convergence behavior above (a/b) and below (c/d) critical $U_c = 6$. Despite error in the updated $V$, all values of converge to within the tolerance, with the except of $U = 6.5$ which terminates after no peaks near $\omega = 0$ were located. The starred points for $U = 2$ and $U = 8$ correspond to the Green’s function evaluations plotted in figure 4 (a) and (b), respectively.

C. DMFT loop

Evaluation of Green’s function and the convergence of the DMFT loop requires minimizing errors and evaluating a series of discrete time points sufficient to determine both the low frequency signal $\omega_1$ and the high frequency signal $\omega_2$. Generally, these two criteria are contradictory to a third consideration of the run-time for the evaluation. That is, increasing the number of shots, the number of randomized Cartan solutions, and the discrete time points evaluated corresponds to increasing accuracy in convergence but significantly increased run-time. Above the critical $U_c = 6$, the frequency $\omega_1$ and the corresponding amplitude $\alpha_1$ converge to 0 at self-consistency. Consequently, for any set of discrete time steps $t_H$ with a nyquist frequency above the high frequency $\omega_2 = \frac{\pi}{2}$ at self-consistency, sampling to a sufficiently long time to distinguish the low frequency signal $\omega_1$ is prohibitively expensive. For example, finding $\omega_1 = .01 \pm .005$ with $U = 8$ requires over 5,000 evaluations using a sampling rate equal to twice $\omega_2$. Instead, we sample Green’s function at two different rates to evaluate $\omega_2$ and then $\omega_1$. Due to frequency aliasing, the order of the sampling is important. Choosing a low sampling rate to accurately evaluate the low frequency $\omega_1$ may result in sampling below the nyquist rate of $\omega_2$, the high frequency signal. For a given sampling rate $\omega_s$, the alias frequency $\omega_a$ can be calculated from the true signal frequency $\omega$ using the following simple formula [44].

$$\omega_a = \left| \omega - \omega_s \times \text{NINT} \left( \frac{\omega}{\omega_s} \right) \right|,$$

where $\text{NINT}(x) \equiv \lfloor \lceil x \rceil / 2 \rceil$ is the (round-half-up) nearest integer to $x$. Thus, we evaluate $\omega_2$ first so the high frequency aliased signal appearing in the low frequency sampling regime can be discarded.

Figure 4 shows the evaluation of $iG(t)$ in the ideal case in orange (i/ii upper) and the results from high frequency sampling for $\omega_2$ in purple (i, lower) and $\omega_1$ in blue (ii, lower). In each case, $t_H$ and $t_L$ are sets of 150 values for time and are chosen with sampling rates between three and ten times greater the than the frequency of $\omega_2$ and $\omega_1$ determined in the previous iteration of the DMFT loop (in both cases above the nyquist rate).

To prevent erroneous updates of the loop when an incorrect peak is found due to noise, only the frequency region around an expected peak, as determined by the previous $\omega_1$ and $\omega_2$ calculation, is searched for peaks. Additionally, each evaluation $iG(t_L)$ and $iG(t_H)$ has a condition to fail for not enough (0) or too many (>4) prominent frequency peaks present in the DFT, as determined by an adaptive height criteria based on the average and standard deviation.
V. RESULTS

Despite significant noise, the quasi-particle and Hubbard band frequencies are preserved in the final discrete Fourier transform of the Green’s function evaluation, allowing for reasonable updates to the DMFT loop, as shown in figure 5. The analytical convergence [45], which is interpolated to serve as a guideline, is compared to the behavior of the convergence of the identical algorithm on a noiseless simulator and the results on quantum hardware. In the insulating phase, even on the noiseless simulator, our algorithm fails to converge exactly to zero for $\omega_1$ due to the vanishing amplitude of $\alpha_1$. Despite significant deviations from the ideal convergence behavior and sequential updates, the convergence on the quantum hardware trends toward self-consistency. In the case of $U = 6.5$, these deviations serve to increase the rate of convergence, but generally the deviations prevent ideal, sequential convergence in spite of the significant filtering and error mitigation.

Figure 6 shows the phase diagram of the quasi-particle weight $Z_{\text{noisy}}$ produced on quantum hardware, plotted against the exact self-consistent solutions for $Z_{\text{exact}}$ [36]

$$Z_{\text{exact}} = \begin{cases} \frac{36 - U^2}{36}, & U < U_c = 6 \\ 0, & U \geq 6 \end{cases}$$

(19)
For all values of $U$, the initial value of $V = 0.5$ is used and the color gradient shows the convergence toward the final value $V_{\text{noisy}}$, which is taken to be the average of the final two steps in the loop. For $U < U_c$, the convergence is within the tolerance $|V_{\text{noisy}} - V_{\text{ideal}}| < 0.02$ at self-consistency for $V$. For $U > U_c$, $\alpha_1$ and $\omega_1$ both vanish to zero, requiring both very long time simulation and a very good signal-to-noise ratio in the results to determine convergence. $Z$ instead converges to above zero but still clearly shows the phase transition. In this regime, the fast-forwarding allowed by Cartan decomposition is essential to appropriately study the dynamics over very long times. Results for $U$ near $U_c$ are omitted, as critical slowing prevents convergence within a reasonable number of iteration steps. The CNOT error and coherence time values for $ibmq\_manila$ can be found in appendix D.

VI. CONCLUSION

Here, we have implemented a two-site DMFT calculation on current generation superconducting quantum hardware with linear CNOT connectivity. Compared to previous methods using Trotter simulation to converge in the insulating phase and variational methods to converge in the conducting phase, our work is the first general implementation to compute the entire DMFT phase diagram \cite{9, 10}. We find that the bottlenecks in the calculation are the noise in the quantum computer and slow convergence near the transition point. To circumvent these issues we introduced a variety of optimization and error mitigation methods including randomized Cartan solutions in the time evolution, measurement error mitigation, analysis of alias signals in the DFT, and post selection of data. The post selection of data includes enforcement of particle number and total spin conservation since the Hamiltonian under consideration cannot create/destroy particles or flip the spin of particles.

Cartan decomposition as a means of fast-forwarding time evolution serves to preserve frequency information despite significant noisy operation in the quantum computer, as demonstrated in this work. Although the algorithm used scales poorly with the number of lattice sites in models of interacting fermions, in such a four-qubit simulation the depth of the algorithm, although significantly longer than a single Trotter step, does not introduce additional numerical errors to the already noisy simulation results and provides access to simulations over much longer time scales than approximations with error scaling in time. Thus, for calculations which depend on oscillation frequencies, such as the DMFT and other embedding problems, this and other fast-forwarding algorithms may prove valuable in the near term, especially when tailored for hardware connectivity.

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DATA AVAILABILITY

The data that support the findings of this study are available from the authors upon request.

Appendix A: Jordan-Wigner transformation

For digital quantum simulation of fermionic systems, we generally map the fermionic algebra of fermion creation and annihilation operations for $n$ fermion modes to the qubit algebra of $n$-qubit Pauli strings $\bigotimes_{l=0}^{n-1} \hat{a}_l^{\dagger}$ ($a_l \in \{x, y, z, 0\}$), which are Kronecker tensor products of the Pauli matrices $\hat{\sigma}^x = X = \left( \begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right)$, $\hat{\sigma}^y = Y = \left( \begin{array}{cc} 0 & -i \\ i & 0 \end{array} \right)$, and $\hat{\sigma}^z = Z = \left( \begin{array}{cc} 1 & 0 \\ 0 & -1 \end{array} \right)$.
and the identity matrix $\hat{\sigma}^0 = I = (\frac{1}{\hbar} \hat{0})$. We introduce the notation $\hat{\sigma}_1^\alpha = I^{\otimes (l-1)} \otimes \hat{\sigma}_1^\alpha \otimes I^{\otimes (n-l)}$ for the type of Pauli strings acting on only a single qubit. For example, $Z_l = \hat{\sigma}_1^\alpha = I^{\otimes (l-1)} \otimes Z \otimes I^{\otimes (n-l)}$. The Jordan-Wigner transformation [46] used in this work provides one such mapping between the fermionic and qubit algebra. The details of the Jordan-Wigner transformation are as follows.

First, map the indexed fermionic states in the Fock basis to indexed qubit states in the computational basis. We employ a mapping where the occupancy numbers of spin↑ modes are as follows:

$$
\text{plugging in equations (A1a) to (A1c) to equation (2) gives}
$$

$$
\hat{H}_{\text{AIM}} = \sum_{i=1}^{N_b} V_i \left( X_0 Z_1 \cdots Z_{i-1} X_i + Y_0 Z_1 \cdots Z_{i-1} Y_i + X_{N_b+i} Z_{N_b+2} \cdots Z_{N_b+i} X_{N_b+i+1} + Y_{N_b+i} Z_{N_b+2} \cdots Z_{N_b+i} Y_{N_b+i+1} \right)
$$

$$
+ \frac{U}{4} (Z_0 Z_{N_b+1} - Z_0 - Z_{N_b+1}) + \sum_{i=0}^{N_b} \frac{\epsilon_i - \mu}{2} (Z_i + Z_{N_b+i+1}).
$$

We have dropped a constant term $\frac{U}{4} I_0 I_{N_b+1} = \frac{U}{4}$ from the above Hamiltonian since a constant energy shift does not affect the dynamics of a system.

For the two-site case, with the impurity site and only one bath site ($N_b = 1$), the Hamiltonian equation (A2) simplifies significantly. Further, at the half-filling (total two particles in the two-site case), $\mu = \frac{U}{2} \epsilon_0 = 0$, and $\epsilon_1 = \frac{U}{2}$ [36, 37]. Therefore, the two-site $\hat{H}_{\text{AIM}}$ with a half-filling ground state is given by equation (3).

**Appendix B: Green’s function evaluation**

Plugging in equations (A1a) to (A1c) to equation (4b) (with $t' = 0$), we obtain

$$
\langle \psi_0 | \hat{c}_0(t)\hat{c}_0^\dagger | \psi_0 \rangle = \langle \psi_0 | U(t) \frac{1}{2} (X_0 + iY_0) U(t) \frac{1}{2} (X_0 - iY_0) | \psi_0 \rangle
$$

$$
= \frac{1}{4} \left[ U(t) X_0 U(t^\dagger) X_0 + i U(t^\dagger) Y_0 U(t) X_0 - i U(t) X_0 U(t) Y_0 + U(t) Y_0 U(t^\dagger) Y_0 \right],
$$

$$
\langle \psi_0 | \hat{c}_0^\dagger(t)\hat{c}_0(t) | \psi_0 \rangle = \langle \psi_0 | \frac{1}{2} (X_0 - iY_0) U(t) \frac{1}{2} (X_0 + iY_0) U(t^\dagger) | \psi_0 \rangle
$$

$$
= \frac{1}{4} \left[ X_0 U(t^\dagger) X_0 U(t) + i X_0 U(t^\dagger) Y_0 U(t) - i Y_0 U(t^\dagger) X_0 U(t) + Y_0 U(t^\dagger) Y_0 U(t) \right],
$$

$$
4iG_{\text{imp}}^R(t > 0) = 4 \langle \psi_0 | \hat{c}_0(t)\hat{c}_0^\dagger + \hat{c}_0^\dagger(t)\hat{c}_0(t) | \psi_0 \rangle
$$

$$
= \langle X_0(t) X_0(t) \rangle + i \langle Y_0(t) Y_0(t) \rangle - i \langle X_0(t) Y_0(t) \rangle + \langle Y_0(t) X_0(t) \rangle + i \langle Y_0(t) Y_0(t) \rangle - i \langle Y_0(t) X_0(t) \rangle + \langle Y_0(t) Y_0(t) \rangle,
$$

(B1)
where $X_0(t) \equiv U^\dagger(t)X_0U(t)$, $Y_0(t) \equiv U^\dagger(t)Y_0U(t)$, $\langle \hat{O} \rangle \equiv \langle \psi_0 | \hat{O} | \psi_0 \rangle$. Measuring the 8 terms in function $G_{\text{imp}}^R(t)$ would require 16 total circuits: two circuits per term for the real and imaginary components, respectively. Using certain symmetries of the impurity Hamiltonian and the ground state we can show that

$$\langle Y_0(t)Y_0 \rangle = \langle X_0(t)X_0 \rangle, \quad \langle Y_0Y_0 \rangle = \langle X_0X_0(t) \rangle. \quad (B2a)$$

$$\langle Y_0(t)X_0 \rangle = \langle Y_0X_0(t) \rangle, \quad \langle X_0X_0 \rangle = \langle Y_0Y_0(t) \rangle. \quad (B2b)$$

Using equations (B2a) and (B2b), we find $4iG_{\text{imp}}^R(t > 0) = 2\langle X_0(t)X_0 \rangle + \langle X_0X_0(t) \rangle = 2\langle X_0(t)X_0 \rangle + \langle X_0X_0(t) \rangle = 4 \text{Re} \langle X_0(t)X_0 \rangle$, which gives equation (5) $iG_{\text{imp}}^R(t > 0) = \text{Re} \langle X_0(t)X_0 \rangle$. This reduces the Green’s function evaluation to a single measurement circuit for $\text{Re} \langle X_0(t)X_0 \rangle$.

Now we prove equation (B2a) first. The impurity Hamiltonian $\hat{H}_{\text{AIM}}$ given by equation (3) is invariant under rotation $R_{z,01} = e^{-i\frac{\pi}{4}(X_0+Z_1)} = e^{-i\frac{\pi}{4}Z_0}e^{-i\frac{\pi}{4}Z_1}$, i.e., $R_{z,01}\hat{H}_{\text{AIM}}R_{z,01}^\dagger = \hat{H}_{\text{AIM}}$, so $[\hat{H}_{\text{AIM}}, R_{z,01}] = [\hat{H}_{\text{AIM}}, R_{z,01}^\dagger] = 0$ and $[U(t), R_{z,01}] = [U^\dagger(t), R_{z,01}] = 0$. Since the ground state $|\psi_0\rangle$ of $\hat{H}_{\text{AIM}}$ is not degenerate and $[\hat{H}_{\text{AIM}}, R_{z,01}] = 0$, $|\psi_0\rangle$ must be the eigenstate of the unitary operator $R_{z,01}$. Therefore, $R_{z,01} |\psi_0\rangle = e^{i\phi} |\psi_0\rangle$, $R_{z,01}^\dagger |\psi_0\rangle = e^{-i\phi} R_{z,01}e^{i\phi} |\psi_0\rangle = e^{-i\phi} R_{z,01} |\psi_0\rangle$, and $\langle \psi_0 | R_{z,01} = \langle \psi_0 | e^{i\phi}$. Now we can prove, for example, $\langle Y_0(t)Y_0 \rangle = \langle X_0(t)X_0 \rangle$.

Similarly, we can prove $\langle Y_0Y_0(t) \rangle = \langle X_0X_0(t) \rangle$.

To prove equation (B2b), we use the time-reversal symmetry of the Hamiltonian $T\hat{H}_{\text{AIM}}T^{-1} = \hat{H}_{\text{AIM}}$. The time-reversal symmetry operator $T = e^{-i\frac{\pi}{4}(\bar{Y}_0 + Y_1 + Y_2 + Y_3)}K = Y_0Y_1Y_2Y_3K$, where the operator $K$ takes the complex conjugation. Similar to $R_{z,01}$ symmetry operator, we have $T |\psi_0\rangle = |\psi_0\rangle$ and $TU(t)T^{-1} = U(-t)$. Beginning with the time-translation invariance result $\langle Y_0(t)X_0 \rangle = \langle Y_0X_0(-t) \rangle$, we prove $\langle Y_0(t)X_0 \rangle = \langle Y_0X_0(t) \rangle$ as follows.

$$\langle Y_0(t)X_0 \rangle = \langle Y_0X_0(-t) \rangle = \langle \psi_0 | Y_0U(t)X_0U(-t) |\psi_0\rangle$$

$$= \langle \psi_0 | T^{-1}(TY_0T^{-1})(TU(t)T^{-1})(TX_0T^{-1})(TU(-t)T^{-1})T |\psi_0\rangle$$

$$= \langle \psi_0 | Y_0U(-t)X_0U(t) |\psi_0\rangle$$

$$= \langle \psi_0 | Y_0U^\dagger(t)X_0U(t) |\psi_0\rangle = \langle Y_0X_0(t) \rangle.$$

Similarly, we can prove $\langle X_0(t)Y_0 \rangle = \langle X_0Y_0(t) \rangle$.

Appendix C: Singular behavior of self-energy and its derivative at zero frequency

We drop the impurity “imp” subscript below for simplicity. Green’s function in the time domain has the form

$$iG(t > 0) = \alpha_1 e^{i\omega t} + \alpha_1 e^{-i\omega t} + \alpha_2 e^{i\omega t} + \alpha_2 e^{-i\omega t} = 2\alpha_1 \cos(\omega_1 t) + 2\alpha_2 \cos(\omega_2 t), \quad (C1)$$

To extract the poles $\omega = \omega_{1,2}$ and pole strength $\alpha_{1,2}$ of the retarded interacting impurity Green’s function, initially take the analytic Fourier transform

$$G(\omega) = \frac{\alpha_1}{\omega - \omega_1} + \frac{\alpha_1}{\omega + \omega_1} + \frac{\alpha_2}{\omega - \omega_2} + \frac{\alpha_2}{\omega + \omega_2}. \quad (C2)$$

The noninteracting Green’s function is given by

$$G^{(0)}(\omega) = \frac{1}{\omega - V} + \frac{1}{\omega + V}. \quad (C3)$$

From the definitions of the self-energy and its derivative, we find:

$$\Sigma(\omega) = \frac{1}{G^{(0)}(\omega)} - \frac{1}{G(\omega)}. \quad (C4)$$
\[
\frac{d\Sigma(\omega)}{d\omega} = -\frac{dG^{(0)}(\omega)/d\omega}{G_2^2(\omega)} + \frac{dG(\omega)/d\omega}{G^2(\omega)} \\
= -\frac{1}{\omega^2} \left\{ \frac{\alpha_1(\omega^2 - \omega_1^2)\omega_1^2 + \alpha_2(\omega^2 - \omega_2^2)\omega_2^2}{2[\alpha_1(\omega^2 - \omega_1^2) + \alpha_2(\omega^2 - \omega_2^2)]^2} - V^2 \right\} + 1 - \frac{\alpha_1(\omega^2 - \omega_1^2)^2 + \alpha_2(\omega^2 - \omega_2^2)^2}{2[\alpha_1(\omega^2 - \omega_1^2) + \alpha_2(\omega^2 - \omega_2^2)]^2} \\
= -\frac{1}{x} \left[ \frac{f(x)}{g(x)} - V^2 \right] + h(x). \\
\]

(C5)

In the last step, we have defined functions \(f(x) = \alpha_1(x - x_2)^2x_1 + \alpha_2(x - x_1)^2x_2\), \(g(x) = 2[\alpha_1(x - x_2) + \alpha_2(x - x_1)]^2\), and \(h(x) = 1 - (\alpha_1(x - x_2)^2 + \alpha_2(x - x_1)^2)/g(x)\), where \(x = \omega^2\), \(x_1 = \omega_1^2\), and \(x_2 = \omega_2^2\), for the discussion below.

Now we derive a stable formula to calculate \(\lim_{\omega \to 0} \frac{d\Sigma(\omega)}{d\omega} = \Sigma'(0)\). First, \(h(x)|_{x=\omega=0}\) is finite because if the denominator of the second term in \(h(x)\) is zero at \(x = \omega^2 = 0\), this implies that \(\alpha_1\omega_2^2 + \alpha_2\omega_1^2 = 0\), which is impossible since \(\alpha_1, \alpha_2, \omega_1, \omega_2 \geq 0\), \(\alpha_1 + \alpha_2 > 0\), and \(\omega_1 + \omega_2 > 0\). Therefore, the first term of \(\Sigma'(\omega)\), \(-\frac{1}{x} \left[ \frac{f(x)}{g(x)} - V^2 \right]\), must also be finite as \(x = \omega^2 \to 0\). This is only possible if \(\frac{f(x)}{g(x)} - V^2 \left|_{x=0} \right. = 0\), which gives

\[
\frac{f(x)}{g(x)} \left|_{x=0} \right. = \frac{f(0)}{g(0)} = \frac{\alpha_1 x_2^2 x_1 + \alpha_2 x_1^2 x_2}{2(\alpha_1 x_2 + \alpha_2 x_1)^2} = \frac{x_1 x_2}{2(\alpha_1 x_2 + \alpha_2 x_1)} = V^2.
\]

(C7)

Therefore, we can evaluate the \(x \to 0\) limit of the first term \(-\frac{1}{x} \left[ \frac{f(x)}{g(x)} - V^2 \right]\) with L'Hôpital's rule as follows.

\[
\lim_{x \to 0} \left[ \frac{f(x)}{g(x)} - V^2 \right] = \frac{g'(0)V^2 - f'(0)}{g(0)} = -\frac{4V^2(\alpha_1 x_2 + \alpha_2 x_1)(\alpha_1 + \alpha_2) + 4V^2(\alpha_1 x_2 + \alpha_2 x_1)(\alpha_1 + \alpha_2)}{g(0)} = 0.
\]

(C8)

Since the first term of \(\Sigma'(\omega)\), equation (C8), is zero, we find

\[
\frac{d\Sigma(\omega)}{d\omega} \left|_{\omega=0} \right. = h(0) = 1 - \frac{\alpha_1 x_2^2 + \alpha_2 x_1^2}{2(\alpha_1 x_2 + \alpha_2 x_1)^2},
\]

(C9)

\[
Z = 1 \left[ \left. 1 - \frac{d\text{Re} \Sigma(\omega)}{d\omega} \right|_{\omega=0} \right] = \frac{2(\alpha_1 x_2 + \alpha_2 x_1)^2}{\alpha_1 x_2^2 + \alpha_2 x_1^2},
\]

(C10)

Equations (C9) and (C10) are more stable and robust against numerical or (quantum) simulation error. The stability comes from the removal of the first term in equation (C5) which is mathematically singular if the condition equation (C7) is not satisfied exactly.

Last, we use the two conditions (derived from the spectral function sum rule \(2\alpha_1 + 2\alpha_2 = 1\) and equation (C7))

\[
\alpha_1 + \alpha_2 = \frac{1}{2}, \quad x_2 \alpha_1 + x_1 \alpha_2 = \frac{x_1 x_2}{2V^2}
\]

(C11a)

(C11b)

to solve for \(\alpha_1\) and \(\alpha_2\) in terms of \(x_1\), \(x_2\), and \(V\), and then eliminate them from the equation (C10). The final result is

\[
Z = \frac{x_1 x_2}{V^2(x_1 + x_2 - V^2)} = \frac{\omega_1^2 \omega_2^2}{V^2(\omega_1^2 + \omega_2^2 - V^2)}.
\]

(C12)

Appendix D: Quantum Hardware

The quantum hardware used in this work was \(ibmq\_manila\), a 5 qubit superconducting device which is publicly available through the IBM Quantum Experience. The experiment parameters are designed around the open access quantum job submission limits of 5 sets of 75 circuit evaluations of 8,192 shots each. Thus, we used two distinct
solutions to the Cartan decomposition which combine to a total shot count of 16,000 at each of 150 time step evaluations. The first set was reserved for just in time measurement error mitigation circuits, of which there are 32 circuits preparing each of the $2^5$ computational basis states. Assuming a correct evaluation, each DMFT Loop requires approximately 36 minutes to execute on the IBM backend, including the Measurement Error Mitigation circuits. In practice, the update failure condition results in repeated calculations and subsequently increased run-times for each $V$ update. Tables I and II show the qubit coherence times and the entangling gate properties, respectively. The ancilla qubit was placed at index 0. Calibration data pulled from the Qiskit API, and averaged by taking the calibration data at 4 points each day between October 10th 2021 and November 10th 2021 [41].

| Qubit Number | T1 ($\mu$s) | T2 ($\mu$s) |
|--------------|-------------|-------------|
| 0 (Ancilla)  | 146.18 ± 29.78 | 94.38 ± 18.50 |
| 1            | 204.64 ± 47.57 | 83.02 ± 15.18 |
| 2            | 148.79 ± 26.79 | 24.30 ± 2.55 |
| 3            | 157.19 ± 36.33 | 63.64 ± 7.83 |
| 4            | 128.96 ± 24.11 | 42.78 ± 2.57 |

**TABLE I:** Average T1 and T2 coherence times for *ibmq_manila*, averaged over the period of time in which runs were executed.

| Connection | CNOT Fidelity | Gate Timing (ns) |
|------------|---------------|------------------|
| 0-1        | 0.0070 ± 0.0012 | 295.11 ± 17.78   |
| 1-2        | 0.0099 ± 0.0017 | 487.11 ± 17.78   |
| 2-3        | 0.0071 ± 0.00080 | 373.33 ± 17.78   |
| 3-4        | 0.0076 ± 0.0016 | 316.44 ± 17.78   |

**TABLE II:** Average CNOT fidelity and gate timings on *ibmq_manila*.

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