Noise-Resilient Quantum Dynamics Using Symmetry-Preserving Ansatzes

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We describe and demonstrate a method for the computation of quantum dynamics on small, noisy universal quantum computers. This method relies on the idea of ‘restarting’ the dynamics; at least one approximate time step is taken on the quantum computer and then a parameterized quantum circuit ansatz is optimized to produce a state that well approximates the time-stepped result. The simulation is then restarted from the optimized state. By encoding knowledge of the form of the solution in the ansatz, such as ensuring that the ansatz has the appropriate symmetries of the Hamiltonian, the optimized ansatz can recover from the effects of decoherence. This allows for the quantum dynamics to proceed far beyond the standard gate depth limits of the underlying hardware, albeit incurring some error from the optimization, the quality of the ansatz, and the typical time step error. We demonstrate this methods on the Aubry-André model with interactions at half-filling, which shows interesting many-body localization effects in the long time limit. Our method is capable of performing high-fidelity Hamiltonian simulation hundred of time steps longer than the standard Trotter approach. These results demonstrate a path towards using small, lossy devices to calculate quantum dynamics.

Introduction. Quantum dynamics was one of the first quantum computing applications envisioned [1] and still remains one of the most promising. Though some quantum devices can be built to specifically simulate the dynamics of a single or small class of quantum systems exactly [2, 3], universal, gate-based quantum computers require some approximate time-stepping scheme. One of the most well-studied is the the Trotter or more generally Trotter-Suzuki decomposition [4], which decomposes the propagator for an arbitrary Hamiltonian into a sequence of gates which can be computed on universal quantum devices. Reaching long times requires gate depths well beyond those achievable on near-term quantum devices [5]. Hybrid quantum-classical methods, especially in quantum chemistry [6–8] and quantum machine learning [9, 10], can alleviate the need for high gate depth by using variational methods with much shorter circuits. There have been proposals for using variational methods to do quantum dynamics on quantum computers, relying on variational principles [11] or subspace expansion [12], which can provide the dynamics of a variational wavefunction using short circuits, but they require an extra, all-to-all connected qubit which computes the derivatives with respect to the variational parameters [13] or are limited to the dynamics of the ground and low-lying excited states [12]. Another recent method uses variational diagonalization to allow for variational fast forwarding of the dynamics [14].

In this Letter, we describe an algorithm for simulating quantum dynamics on small, noisy, universal quantum computers using the idea of restarting the dynamics after each time step. In order to advance a wavefunction from time $t$ to $t + \Delta t$, a Trotter time step is first carried out on the quantum hardware. Rather than continuing the propagation, a variational ansatz is fit to the result and this ansatz is used for the next time step. By including knowledge of the form of the solution directly into the ansatz, such as the symmetries it must obey, this procedure provides a significant resilience to decoherence, allowing for much longer propagation times with high fidelity. We demonstrate the method on multiple instantiations of the Aubry-André model with interactions at half-filling, using simulations of noisy quantum computers with various levels of decoherence. Our restarted quantum dynamics (RQD) algorithm is able to maintain a high-degree of fidelity (>0.9) for hundreds of time steps after the standard Trotter approach has lost all coherence and reached fidelities of zero. We show that, when using RQD, even a near-term quantum computer will be able to prepare interesting, many-body localized states.

Method. Let $H$ be some Hamiltonian and $|\psi(t)\rangle$ be the true wavefunction at some time $t$. We seek the dynamics of the wavefunction given initial condition $|\psi(0)\rangle$. Rather than propagate all time steps on the quantum computer directly, we propose to instead “restart” the dynamics after each time step by optimizing a wavefunction to approximate the time-stepped wavefunction. We make use of a parameterizable circuit, $C(\theta)$, giving a wavefunction

$$|\psi(\theta)\rangle = C(\theta)|0\rangle,$$

where $\theta$ is a set of parameters, such as rotation angles, of a circuit and $|0\rangle$ is the initial all zeros state of the quantum computer. We take at least one time step directly on the quantum computer via, e.g., a Trotter-like procedure. We then optimize the parameters of a new wavefunction, $|\psi(\theta_n)\rangle$, to the time-stepped wavefunction, solving the following optimization problem

$$\min_{\theta_n} \left(1 - |\langle\psi(\theta_n)|\psi(t + \Delta t)\rangle|^2\right)^2,$$

where $|\psi(t + \Delta t)\rangle$ is the time-stepped wavefunction. The RQD method is shown schematically in Fig. 1(a).

The proposed algorithm can be summarized as three basic steps: 1) prepare the wavefunction $|\psi(t)\rangle$, which
may itself be a circuit with a set of optimal parameters found in a previous iteration; 2) take a single Trotter time step directly on the quantum computer; 3) optimize the fidelity of the time-stepped wavefunction with time step directly on the quantum computer; 2) take a single Trotter step twice and take a single Trotter time step (see Fig. 1(b)), this method can be ‘restarted’ many times. To demonstrate this, we use the Aubry-André model with interactions at half-filling, a prototypical Hamiltonian which can demonstrate many-body localization.

**Aubry-André Model.** Here, we study the one-dimensional spinless Aubry-André model with interactions, given by the Hamiltonian

$$H = -J \sum_{k=1}^{N} (a_k^\dagger a_{k+1} + a_{k+1}^\dagger a_k) + h \sum_{k=1}^{N} \cos(2\pi \beta k + \phi) a_k^\dagger a_k + U \sum_{k=1}^{N} a_k^\dagger a_k a_{k+1}^\dagger a_{k+1}, \quad (3)$$

where $N$ is the number of sites, $J$ is the hopping strength, $h$ is the disorder strength, $\beta$ is an irrational number, $\phi$ is a phase offset, $U$ is the interaction strength, and we impose periodic boundary conditions. The second term describes the disorder, which can be described by the interaction of two lattices with a ratio of periodicities $\beta$ and phase offset $\phi$ \[10\]. For almost all irrational $\beta$, the Aubry-André model shows interesting localization effects \[19\]. This model is shown schematically in Fig. 1(c). Methods using matrix product states can efficiently evolve such systems for short times, but the entanglement grows as the dynamics proceeds, due to the fact that dynamics involves many excited, entangled states \[20\], increasing the necessary bond dimension \[21\]. Since quantum computers live within the full Hilbert space, they can naturally represent such highly entangled superpositions.

One example of an interesting dynamical quantity is the breaking of ergodicity due to many-body localization, which has been demonstrated experimentally for small numbers of spins \[22\]. Starting from an initial charge density wave where even sites are unoccupied and odd sites are occupied, $|\psi(0)\rangle = |1, 0, 0, 0, 0, 0, 0, 0\ldots\rangle$, the evolu-

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**FIG. 1:** (a) Diagram of restarted quantum dynamics (RQD) method. Blue shading represents steps taken on the quantum computer; yellow shading represent steps taken on the classical computer. (b) An example of a circuit used in the RQD method to estimate the fidelity between the time-stepped wavefunction and the new wavefunction ansatz. (c) Diagram of Aubry-André model with interactions.
tion of the imbalance,

\[ I(t) = \frac{N_e(t) - N_o(t)}{N_e(t) + N_o(t)}, \]

where \( N_e(t) \) is the occupation of even sites and \( N_o(t) \) is the occupation of odd sites. A nonzero imbalance at long times implies that the state is many-body localized \[23\].

Results. Using simulations of noisy quantum computers, we calculate the dynamics of many instantiations of the Aubry-André model with interactions, fixing \( \beta = \sqrt{2}, \frac{\mu}{J} = \frac{\hbar}{J} = 4, \) and choosing \( \phi \) randomly from a uniform distribution in the range \([0, 2\pi]\). We compare three different strategies for calculating the dynamics: Trotter, where we apply the Trotterized evolution circuit multiple times, and the RQD method with two different ansatzes. The first ansatz is a number-conserving circuit which, for any value of the parameters, conserves the total particle number \[24\]. Since the Aubry-André model conserves total particle number, this number-conserving ansatz directly builds in an important symmetry of the Hamiltonian. The second ansatz is an idealized, ‘oracle’ ansatz of the form \( C(\theta) = \exp(-i\theta H) \), which is the true propagator with the time as the single parameter and has all of the possible symmetries of the Hamiltonian. We use a time step of \( \Delta t = 0.04 \) in all instances. We minimize Eq. (2), which maximizes the fidelity, using L-BFGS \[24\] with numerical gradients up to a tolerance of \(10^{-12}\) or for a maximum of 80 iterations. Analytical gradients could also be calculated directly on the quantum computer by various means, such as shifting the rotation angles by specific values \[20\].

We simulate the evaluations of these circuits on a noisy quantum computer at various noise rates using the density matrix master equation formalism \[27, 28\], as implemented in the high-performance quantum dynamics simulator, QuaC \[29\]. Noise is modeled using both environmental amplitude-damping (\( T_1 \)) and pure dephasing (\( T_2^* \)) noise. Gates are treated as perfect, unitary operations which happen at a time \( t \) and are followed by a wait time consistent with the gate times of IBM’s superconducting qubit quantum computers (100-1000ms) \[8\]. We treat the oracle ansatz as a single gate which takes the same amount of time as the whole of the number-conserving ansatz, namely 0.026ms. Due to variance in the effectiveness of the compilation and scheduling, the evolution circuits take between 0.102ms and 0.245ms per time step. Since we use the density matrix formalism, we have no stochastic sampling errors. Additional details about the generation of the evolution circuits and the noisy quantum computer simulations can be found in the appendix.

Fig. 2 shows the calculated imbalance for two specific instantiations of \( \phi \), as well as the average over all 16 calculations on a simulated noisy quantum computer with \( T_1 = T_2^* = 25\)ms. The average propagation circuit over all \( \phi \) values compiles to 0.160ms per time step. Roughly, this implies that a standard Trotter procedure could take between 10 and 20 time steps before the total circuit time exceeds a tenth of the coherence time of our simulated quantum computer and the noise effects would begin to greatly affect the output. This can be seen clearly in Fig. 2. In the shorter circuit, with \( \phi = 3.2627696 \) and a propagation circuit length of 0.147ms per time step, the standard Trotter procedure is able to weakly capture one oscillation at around \( t = 2 \), after 50 time steps and a total propagation time of around 8ms. In the longer circuit, with \( \phi = 5.64240529 \) and a propagation circuit length of 0.245ms, the standard Trotter procedure decays much faster, only capturing a hint of the first oscillation.

The RQD method, on the other hand, quantitatively captures the dynamics for the whole time window calculated. For the shorter circuit of \( \phi = 3.2627696 \), the number-conserving ansatz is able to capture most of the broad oscillations and even many of the smaller oscillations, whereas in the longer circuit of \( \phi = 5.64240529 \), it captures only the broad oscillations. The oracle ansatz, on the other hand, captures essentially all of the features. The oracle ansatz encodes all of the possible symmetries of the wavefunction, whereas the number-conserving ansatz only has the single, but important, particle number symmetry. This allows the oracle ansatz to effectively recover from more errors than the number-conserving
ansatz. The oracle ansatz is also much simpler to optimize, having only a single parameter, compared to the 38 parameters of the number-conserving ansatz, allowing it to reliably converge to our optimization tolerance of $10^{-12}$. The number-conserving ansatz almost always reached the iteration limit before converging.

The lower panel of Fig. 2 shows the average imbalance over all 16 $\phi$ values. The parameters of the Aubry-André model we chose ($J = J' = 4$) are beyond the critical disorder strength ($\frac{J}{J'} = 2$) for localization. As such, the true dynamics show a significant nonzero imbalance at long times. For both ansatzes, the RQD method agrees well with the true dynamics, showing the many-body localization effect. The Trotter dynamics, on the other hand, only reproduces the correct imbalance before $t = 1$. In the longer times, the imbalance has decayed to 0, and the many-body localization effect is not observable.

Figure 3 shows the average fidelity over all 16 values of $\phi$ at different $T_1 = T_2$ coherence times for the time slice $t = 5$. At very long coherence times (very low noise rates), including the noise-free case, the standard Trotter procedure performs better than RQD with the number-conserving ansatz, but worse than the oracle ansatz. The oracle ansatz even recovers from Trotter errors, as it can only prepare states that are part of the true dynamics. The number-conserving ansatz, on the other hand, is a more flexible wavefunction that can, in principle, fit the Trotter wavefunction, even with Trotter errors. It performs worse than Trotter for long coherence times due to the optimization failing to converge to a small enough tolerance. As the coherence times decrease (and the noise rates increase), the fidelity of the standard Trotter procedure drops quickly, going to nearly zero at a coherence time of only 25ms. The oracle and number-conserving ansatzes both maintain high fidelity at 25ms. In fact, the fidelity of RQD with either ansatz is competitive with the standard Trotter procedure at coherence times two orders of magnitude smaller.

The inset of Fig. 3 shows the average fidelity over all 16 values of $\phi$ for the coherence time $T_1 = T_2 = 25$ms throughout the calculation of the model dynamics. The average fidelity of the standard Trotter procedure quickly drops off as more time steps are taken due to the increasing circuit depth. The RQD method, with either ansatz, maintains a high fidelity. The oracle ansatz maintains a fidelity of nearly 1, whereas the number-conserving ansatz decays slowly. The oracle ansatz encodes far more symmetries than the number-conserving ansatz, making it inherently more robust to more types of errors. For example, pure dephasing errors, which are parameterized by $T_2^*$, can maintain particle number but still cause the fidelity to decrease. The number-conserving ansatz is, therefore, not robust to these errors and they gradually build up as the calculation proceeds. This is in addition to errors from optimization, which also gradually build up. When the optimization terminates due to reaching the iteration limit, the next time step comes from a wavefunction which approximates the time-stepped wavefunction worse than otherwise possible, leading to a build up of error as more time steps are taken. One way to mitigate the build up of such optimization errors as quantum computers with longer coherence times are built is to take multiple Trotter time steps before the restart procedure. Utilizing recent advancements in error mitigation techniques, such as error extrapolation [11, 30–33], could help allow multiple Trotter time steps to be taken.

The key overhead of the RQD method is optimization. For realistic ansatzes, such as the number-conserving ansatz used here, the number of parameters will generally be large and the number of iterations needed for convergence will also become large. Even though each function evaluation involves measuring only a single observable, the fidelity, there is need for algorithmic improvement in the optimization subroutine to ensure the method remains practical for large systems. Recent advancements in optimization for other hybrid quantum-classical methods [34, 35] can be applied to restarted quantum dynamics to alleviate this overhead. Furthermore, efficient ansatz design, which is problem specific, could restrict the number of free parameters, providing more robustness to noise and additional ease of optimization.

Conclusion. We described and demonstrated an algorithm for carrying out dynamics calculations on lossy, near-term quantum computers using the idea of “restarting” the dynamics. This restarting procedure involves approximating the time-stepped wavefunction with some variational ansatz which is optimized to give the result of the time step. By encoding known symmetries of the true wavefunction into the ansatz, the RQD method is able to mitigate the effects of noise during the propagation at the additional cost of optimization. Careful ansatz design
PILE the resulting circuit for a fully-connected quantum Trotter procedure \([4]\), with time step \(\Delta t\). Then generate the evolution operator using a first-order OpenFermion \([37]\), to obtain the qubit Hamiltonian. We apply the Jordan-Wigner transform \([36]\), using \(\varphi\).

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### Propagation Circuit Generation

We first generate the fermionic Hamiltonian for a given \(\phi\) and apply the Jordan-Wigner transform \([36]\), using OpenFermion \([37]\), to obtain the qubit Hamiltonian. We then generate the evolution operator using a first-order Trotter procedure \([4]\) with time step \(\Delta t = 0.04\), and compile the resulting circuit for a fully-connected quantum computer using Qiskit \([38]\). Due to differences in the compilation and scheduling procedures (see below), the resulting circuits end up with different final numbers of layers. The sixteen values of \(\phi\) and the resulting circuit lengths are shown in Table I.

| \(\phi\)          | Total Time (ms) | Layers | Gates |
|-------------------|-----------------|--------|-------|
| 1.93146731        | 0.1158          | 163    | 187   |
| 5.64240529        | 0.2452          | 312    | 347   |
| 1.57973617        | 0.1602          | 212    | 246   |
| 0.08769829        | 0.2264          | 291    | 324   |
| 4.42879993        | 0.1642          | 219    | 251   |
| 1.59366522        | 0.1822          | 238    | 270   |
| 1.69972758        | 0.1494          | 203    | 230   |
| 3.26279226        | 0.1472          | 197    | 223   |
| 6.09740422        | 0.2302          | 294    | 329   |
| 3.34406920        | 0.2632          | 335    | 372   |
| 3.26279660        | 0.1026          | 148    | 170   |
| 4.52159699        | 0.2102          | 274    | 308   |
| 2.94545992        | 0.1522          | 203    | 234   |
| 4.71502552        | 0.2184          | 283    | 314   |
| 1.08255072        | 0.2122          | 274    | 306   |
| 4.85940981        | 0.1022          | 146    | 172   |

TABLE I: Values of \(\phi\) and the time, number of layers, and total number of gates for the corresponding evolution circuits.

which includes a priori knowledge is necessary to provide the noise mitigation. A completely flexible ansatz would learn the noise effects, along with the dynamics. We demonstrated that RQD with only number-conservation symmetry in the ansatz was able to greatly extend the length of calculation of the Aubry-André model with interactions that could be computed on a simulation of a noisy quantum computer. At a coherence time of \(T_1 = T_2^* = 25\) ms, the RQD approach was able to take hundreds of time steps beyond where the standard Trotter procedure began to fail. With additional symmetries, RQD performs even better. Restarted quantum dynamics is a promising algorithm that could pave the way for quantum dynamics calculations on quantum computers which take many more time steps than the coherence time would naively allow.

### Scheduling Algorithm

We use a simple, greedy algorithm to schedule the gates into layers where all gates can be applied in parallel. The algorithm begins with a list of gates which are guaranteed to be in correct sequential order. We also initialize the current layer counter for each qubit to zero. In sequence, we check the qubits to which each gate is applied. We assign the current gate to the maximum of the current layers for the constituent qubits. We then set the current layer counter of the constituent qubits to the maximum of the current layers plus one. This process is done until all gates have been assigned layers. The layers are then applied in sequence, with layers potentially being comprised of multiple, parallel gates.

### Simulation of Noisy Quantum Computer

We use the Lindblad master equation to simulate a noisy quantum computer. The Lindblad master equation for a general system is

\[
\frac{d\hat{\rho}}{dt} = -i\frac{\hbar}{\hbar}[\hat{H}, \hat{\rho}] + L(\hat{\rho}),
\]

where \(\hat{H}\) is the system Hamiltonian and \(L(\hat{\rho})\) is the Lindblad superoperator describing decoherence effects. For our system, we use no direct Hamiltonian \(\hat{H}\) and we simulate amplitude-damping (\(T_1\)) and pure-dephasing (\(T_2^*\)) decoherence sources,

\[
L_i(\hat{\rho}) = -\frac{1}{2T_1}(\hat{\sigma}_i^\dagger \hat{\sigma}_i \hat{\rho} + \hat{\rho} \hat{\sigma}_i^\dagger \hat{\sigma}_i - 2\hat{\sigma}_i \hat{\rho} \hat{\sigma}_i^\dagger) - \frac{1}{2T_2}(\hat{\sigma}_i^\dagger \hat{\sigma}_i \hat{\rho} + \hat{\rho} \hat{\sigma}_i^\dagger \hat{\sigma}_i - 2\hat{\sigma}_i \hat{\rho} \hat{\sigma}_i^\dagger),
\]

where \(L_i(\hat{\rho})\) is the Lindblad superoperator for qubit \(i\), \(\hat{\sigma}_i\) is the annihilation operator for qubit \(i\), and all qubits have the same coherence times, \(T_1\) and \(T_2^*\).

### Number Conserving Ansatz

Figure 4 shows the explicit number-conserving ansatz used in the main text, using the ‘A’ gate of figure 5. This ansatz conserves three particles within six sites. It was generated according to the method of [24].

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$A(\theta_1, \theta_2) = R_z(-\theta_1) R_y(-\theta_2) R_y(\theta_2) R_z(\theta_1)$

FIG. 4: Number-conserving ansatz for three particles in six sites.

$A(\theta_3, \theta_4) = R_z(-\theta_3) R_y(-\theta_4) R_y(\theta_4) R_z(\theta_3)$

FIG. 5: ‘A’ gate used in number-conserving ansatz.
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