IBM Quantum Awards: Open Science Prize Submission

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April 22, 2022

Abstract

We present our submission for the IBM Quantum Open Science Prize, which focuses on the simulation of the XXX Heisenberg spin model on real quantum hardware. The keystone of our approach is the use of Incremental Structural Learning (ISL), a quantum algorithm for approximate circuit recompilation, to find circuits that produce approximately the same state as the desired time evolution circuit with significantly fewer gates. The trial solution is built and optimised incrementally, with the structure of each layer informed by the entanglement properties of the original circuit. Our open-source implementation, built as part of this challenge, is available at `https://github.com/abhishekagarwal2301/isl/`.

Combining this method with measurement calibration, we achieve a 99.3% fidelity on the tomography benchmark for the evolved state at $t = \pi$. Furthermore, to demonstrate the general applicability of our solution beyond this special case, we reconstruct the probability of the $|110\rangle$ state across the entire range $t = (0, \pi)$ on *ibmq_jakarta*. Excitingly, despite the more complicated entanglement spectrum of the system at these intermediate times, our results match the form of the analytic solution, producing a probability on average within 2.4 percentage points of the true value.

These notes supplement the Jupyter notebook entitled `ibmq-qsim-challenge-main.ipynb`, which together make up our entry into this year's Open Science Prize. We'd like to thank the organisers for running the challenge, which we have enjoyed grappling with and trying to solve. We hope you enjoy our solution as much as we enjoyed making it.

Our attempt to solve the Trotterised evolution problem consists of two key error mitigation techniques: approximate quantum circuit recompilation (AQCR) and measurement calibration. Whilst the latter is well established, it is the former which generally has not seen widespread use as a tool that can drastically reduce the noise generated when running quantum circuits. As such, the main focus in this supplement is to give a background to AQCR as well as more details of the Incremental Structural Learning (ISL) algorithm.

This document is laid out as follows. First, we introduce and describe AQCR, including its formulation as an ansatz problem. Subsequently we detail how ISL circumvents this problem by iteratively learning shallower approximate equivalents of quantum circuits through the process of disentangling them - and why it is particularly good for Trotterised evolution. Finally, we make clear the novel contributions of our submission as well as a description of the key results obtained in case of failures with the Jupyter notebook.

A final note: the ideas presented in our submission and the ISL algorithm itself is the culmination of an effort started by AA and BJ over 2 years ago and has been in the public domain since 2020 [1]. In that initial work, an alpha version of ISL was tested as an error mitigation tool on fake noisy devices. The announcement of the IBM Quantum Awards 2021, with the harder challenge of obtaining Trotterised evolution on a *real device*, encouraged us to improve ISL and attempt to apply it as a solution to simulating the XXX model. In the spirit of the Open Science Prize, we consider a significant part of our submission to be the building of an open source ISL library, which we hope can be used and further extended by others in the field.

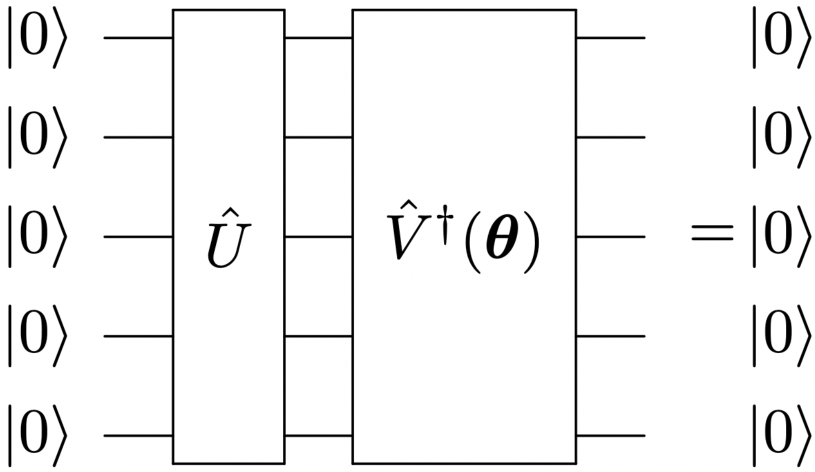

Figure 1: In approximate quantum circuit recompilation, the problem of finding a set of gates $\hat{V}$ that approximates the action of another circuit $\hat{U}$ on an initial state can be considered as finding the inverse $\hat{V}^\dagger$ that recovers the initial state. As the form of the inverse is unknown, a parameterised ansatz $\hat{V}^\dagger(\boldsymbol{\theta})$ is optimised to try and achieve this. For an initial state $|0\rangle^{\otimes n}$, ISL avoids guessing a fixed structure of the ansatz and instead incrementally builds two-qubit layers with aim of disentangling the circuit back to a product state.

Background [1]

Given a unitary $\hat{U}$, quantum circuit compilation describes the process of finding an implementation of $\hat{U}$ on a quantum computer using a series of m gate operations. On the other hand, quantum circuit *re*compilation is the process of trying to improve an existing circuit by replacing it with a circuit that generates the same unitary but takes less time to run. This is important for current quantum computers, whose short-lived qubits rapidly undergo decoherence, creating noise, and as such quantum circuit re-compilation can be viewed as a error mitigation technique. Furthermore, if we recompile a circuit without knowledge of individual gate times, we can reformulate the problem generally as finding a circuit which implements $\hat{U}$ in $o < m$ gate operations. Solutions to this range from duplicate gate cancellation [3] to two-qubit block re-synthesis [4] involving the KAK decomposition [5].

In this submission we utilise recent advances in approximate circuit recompilation. Here, rather than find an exact alternative implementation of $\hat{U}$, the goal is to find a shallower quantum circuit $\hat{V}$ which has approximately the same action on some initial state $\hat{U}|\psi\rangle \approx \hat{V}|\psi\rangle$. Reformulating this as $\langle\psi|\hat{V}^\dagger\hat{U}|\psi\rangle \approx 1$, we notice that the problem can be viewed as finding the set of gates $\hat{V}^\dagger$ that inverses the action of $\hat{U}$ as measured by the overlap between the initial and final state, to within some desired accuracy. Once the inverse is found, each gate that makes up $\hat{V}^\dagger$ can be inverted to produce our desired approximately equivalent circuit $\hat{V}$. This process of trying to find the inverse can itself be recognised as an energy minimisation problem, leading to the popular approach to solve it with a variational quantum algorithm [6, 7, 8]. However, like many variational algorithms, the best solution often requires finding the optimal ansatz through a potentially lengthy trial-and-error process. Furthermore, what constitutes the best ansatz may vary dramatically for different inputs, such that training multiple ansatzes for every circuit to be recompiled dramatically increases the complexity of general AQCR. Attempts to use a single problem-agnostic ansatz for multiple inputs would require the ansatz to have a random structure, leading to trainability issues imposed by barren plateaus [9]. These limitations combined are what we consider to be *the ansatz problem* for AQCR.

[1] Parts of this section are borrowed from a recent preprint [2] which was developed in tandem with this submission, as well as the original ISL paper.

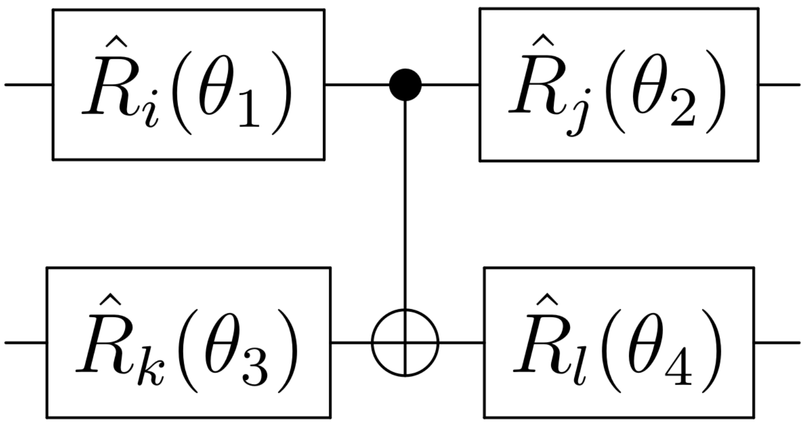

Figure 2: A thinly-dressed CNOT gate is a CNOT gate surrounded by 4 single-qubit rotation gates $\hat{R}_i(\theta)$, where $i \in \{x, y, z\}$ is the axis of rotation and θ is the angle.

ISL solves the ansatz problem

ISL attempts to solve this problem by exploiting structure in the initial state and using it to guide the building of the ansatz $\hat{V}^\dagger$. Firstly, if the initial state is $|\psi_0\rangle = |0\rangle^{\otimes n}$ as is convention for quantum algorithms, then we note that the problem can be expressed as findings the set of gates that maps the original circuit $\hat{U}$ back to $|\psi_0\rangle$. This particular formulation of the problem is shown in Fig. 1. Notably, our target state is a product state, with no entanglement between the qubits. Thus, any ansatz we build should focus on adding gates that work to disentangle the state produced by $\hat{U}$.

Secondly, instead of using a fixed ansatz for $\hat{V}^\dagger$, we incrementally build its structure layer-by-layer, evaluating the cost function $C = 1 - \left|\langle\psi_0|\, \hat{V}^\dagger \hat{U}\, |\psi_0\rangle\right|^2$ each time. This approach offers the greatest flexibility to find the optimal solution and follows other notable successes using incrementally built ansatzes [10], whilst also avoiding the issue of barren plateaus.

Combining the above two points we reach the essence of the ISL solution for AQCR: incrementally building an ansatz where each layer aims to disentangle the most entangled pair of qubits.

Constructing $\hat{V}^\dagger$

Overall, the ansatz $\hat{V}^\dagger = \hat{V}_n^\dagger ... \hat{V}_1^\dagger$ consists of n layers of $\hat{V}_i^\dagger$, where $\hat{V}_i^\dagger$ is a thinly-dressed CNOT gate as shown in Fig. 2. We describe this as thinly dressed because the single-qubit gate rotations are restricted to one axis - in contrast to the regular dressed CNOT gates in [11]. When adding the i^{th} layer $\hat{V}_i^\dagger$, we must first decide which qubits should be acted on. To do this we evaluate an entanglement measure E between each pair of qubits, which are in the state $\hat{V}_{i-1}^\dagger ... \hat{V}_1^\dagger \hat{A}\, |\psi_0\rangle$. Whilst in [1] only the entanglement of formation [12] was considered, our improved version of ISL for this submission considers additionally concurrence [13] and negativity [14], which can be calculated via the statevector or directly on the quantum circuit. We then pick which qubits will have a thinly-dressed CNOT gate applied in the upcoming layer by the pair with the largest entanglement measure. This completes the addition of the layer $\hat{V}_i^\dagger$.

It is also possible that all qubit pairs have $E = 0$. For example, the maximally entangled state $|GHZ\rangle$ does not have any pairwise local entanglement and will result in $E = 0$ for all qubit pairs. In this case, we measure the expectation value $\langle\hat{\sigma}_z\rangle$ of each qubit. Since $\langle\hat{\sigma}_z\rangle = 0$ for the input qubits, we apply a thinly-dressed CNOT layer to the two qubits with the highest and second highest expectation values. This can be considered as the later refinement stages of ISL, where the input state has been successfully disentangled to a product state, but the output is not yet $|0\rangle^{\otimes n}$.

One constraint that we impose on the choice of the control and target is that it must not be the same as the control and target for the previous layer. This is because in general, adding layers to different choices of control and target qubits allows us to explore a greater region of the available Hilbert space. This also avoids creating circuits with large depth but small numbers of gates. Hence, if the qubit pair with the highest E is the same as in the previous layer, we choose different qubits with the two largest expectation values instead.

Once we have chosen the control and target qubits, we add the layer to $\hat{V}^\dagger$ with initial rotations $\theta = 0$ about the z axis.

Optimising

After a layer is added, the axes and angles of rotation of the single-qubit gates are optimised using the `rotoselect` structural learning procedure [8], with respect to minimising the cost. This procedure works by fixing three of the gates and varying the rotation axes and angle for the remaining one. This is then repeated, sequentially cycling over the 4 rotation gates until a termination criterion is reached. We define this as when the reductions in the cost function between cycles is less than 1%.

Once the single-qubit gates of this particular layer have been optimised, we then optimise the whole ansatz $\hat{V}^\dagger$ using `rotosolve` [8]. This procedure is similar to `rotoselect`, but doesn't involve optimizing the rotation gate axes.

Terminating

Once the `rotosolve` procedure is terminated, we perform standard non-approximate transpilation of $\hat{V}^\dagger$. Examples of this include the removal of both duplicate gates and rotation gates with very small angles.

After this we take one final measurement of the cost function. If it is above a certain minimum threshold, we repeat the process again and add a new layer. If it is below the threshold, we terminate ISL and recursively invert all of the gates in the ansatz to return $\hat{V}$. In the case of simulating the XXX Hamiltonian, this is then our approximate equivalent of the N Trotter step circuit.

Scaling of ISL for intractably large circuits

The ISL routine requires the repeated execution of two different circuits: the target $\hat{U}|\psi\rangle$ and the current best guess of the target plus inverse $\hat{V}^\dagger\hat{U}|\psi\rangle$, where $\hat{V}^\dagger$ contains between 0 and L layers of thinly-dressed CNOT gates. In our submission, these circuits are evaluated on the statevector simulator, done to reduce any noise in the recompilation process itself and find the best solution, which in turn leads to the highest benchmark possible. Clearly however, working directly with the states to calculate the cost function and entanglement metrics is a luxury only afforded when studying classically tractable systems. Here we make it clear that ISL and by extension our submission is scalable to systems that are too large to allow storing the statevector. Although not required by the competition, we have implemented the option for obtaining the entanglement concurrence directly from the circuit [15, 16]. This makes the entire algorithm runnable on a quantum computer without the use of additional qubits, controlled-unitary operations, or full state-tomography. Naturally however, it would be expected that running ISL recompilation on current noisy devices could significantly reduce the accuracy of the solution. Finally, we note that if ISL was run on real noisy hardware, it is clear that we wouldn't be able to evaluate the circuit $\hat{V}^\dagger\hat{U}|\psi\rangle$ accurately, otherwise we would simply run the original $\hat{U}|\psi\rangle$ and do away with recompilation. In the case of simulating quantum dynamics, as we do in this submission, this would be solved by recompiling the evolution operator, Trotter step by Trotter step, laddering the solutions together. This process, sometimes called restarted quantum dynamics [17], would introduce an additional error scaling from the propogation of the cost function.

Novel contributions

Our submission consists of the following novel contributions. Firstly, we consider the use of approximate circuit recompilation underrepresented in the wider context of error mitigation tools, and hope the judges recognise the novelty in this. Instead of post-processing techniques, such as zero-noise extrapolation, we focus on whether structure in the circuit can be exploited to make the circuit itself shallower and generate less noise on the real device. Secondly, we construct an open-source implementation of ISL, accessible at `https://github.com/abhishekagarwal2301/isl/`. Whilst the method is available publicly and has been applied to research problems before [18], the implementation has previously remained in the private domain. Significant effort has been put into the documentation and to try and make our solution easy

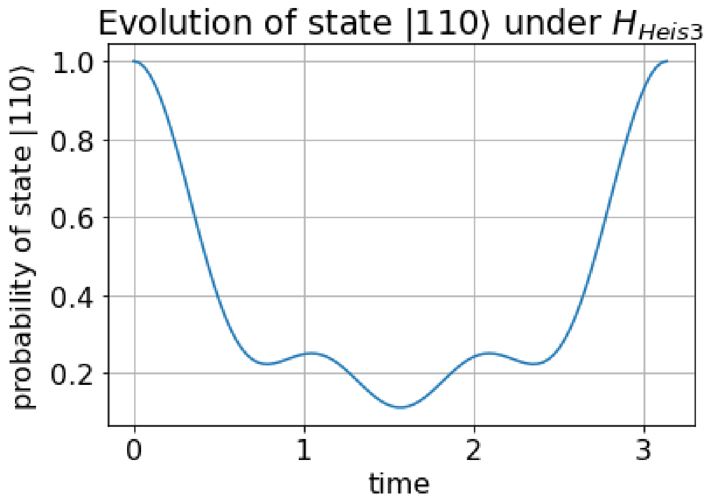

Figure 3: Analytic evolution of the $|110\rangle$ computational basis state under H_{Heis3} as provided by the competition template.

to use, hopefully encouraging others to try and evolve it further. As shown in the README, any circuit can be recompiled (using default settings) with only two lines of code. Finally, our library created for the Quantum Awards has a number of additional features that leads to greater error mitigation than the original algorithm, including:

- Entanglement measures of concurrency and negativity, calculated from the statevector (if using the statevector simulator) or from circuit observables allowing for running on the real device.
- Ability to specify a custom coupling map for the recompiled solution. Whilst not employed in our submission code, this would help when recompiling circuits with significantly different topologies to the real device that we want the recompiled circuit to be run on.
- Evaluation of the overlap $\left|\langle\psi_0|\,\hat{V}^\dagger\hat{U}\,|\psi_0\rangle\right|^2$ not only from the statevector, but also as a SWAP test. This would allow in theory the testing of running ISL on real quantum computers, for intractable sizes beyond what was required in this submission.

Key Results

Here, we present and describe the main results from the Jupyter notebook, in case of an error occurring with it.

In Fig. 3 we arrive at the start of the challenge - the analytic solution to the evolution of the $|110\rangle$ state under the XXX Heisenberg Hamiltonian. Although the benchmark is based on the fidelity achieved after time $t = \pi$, we are going to take the ambitious step of trying to reproduce this whole graph on the real device to the highest possible accuracy we can achieve.

In Fig. 4 we demonstrate the first step of our solution. Taking the provided circuit decomposition, we plot the dynamics obtained across $t = (0, \pi)$ on the qasm simulator when discretising the time into increasing numbers of Trotter steps. Without device errors, we are able to find the minimum number of total Trotter steps required such that the error incurred by the 1st order Trotter decomposition is negligible. Since this threshold is somewhat arbitrary, we take this to be the number of Trotter steps for which we judge visual convergence between the markers and analytic solution. Fig. 4 shows the results of this search, plotting the analytic evolution against the simulated evolution for $n = 35$ Trotter steps.

With the minimum number of Trotter steps ascertained, we present the next step of the solution. Here, we demonstrate the effectiveness of the ISL algorithm to find approximately equivalent circuits that can produce the same states with high fidelity. We recompile each of the Trotter step circuits in Fig. 4 using ISL with a sufficient cost of 10^{-3}, setting the minimum overlap threshold between the states produced by the original and recompiled circuits to be 99.9%. Fig. 5 shows the result of executing each of these

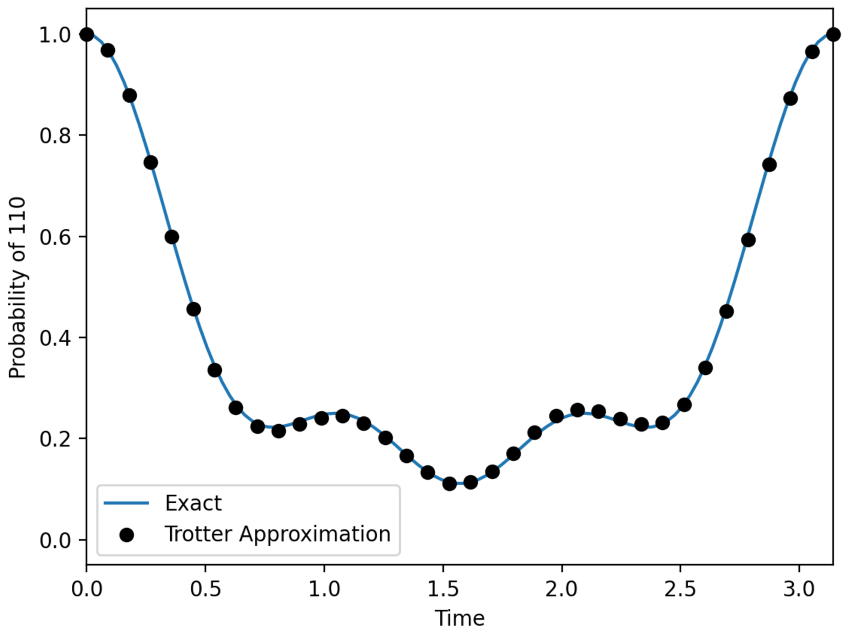

Figure 4: Probability of measuring the $|110\rangle$ computational basis state as obtained analytically (blue line) or using a Trotterised circuit decomposition (black circles) obtained on the Qiskit statevector simulator. The single Trotter step circuit is repeated between $n = 1$ to $n_{\max} = 35$ times to build up the markers. Notably, by discritising the time into $n_{\max} = 35$ slices, the Trotter error is small enough to allow for convergence with the analytic solution

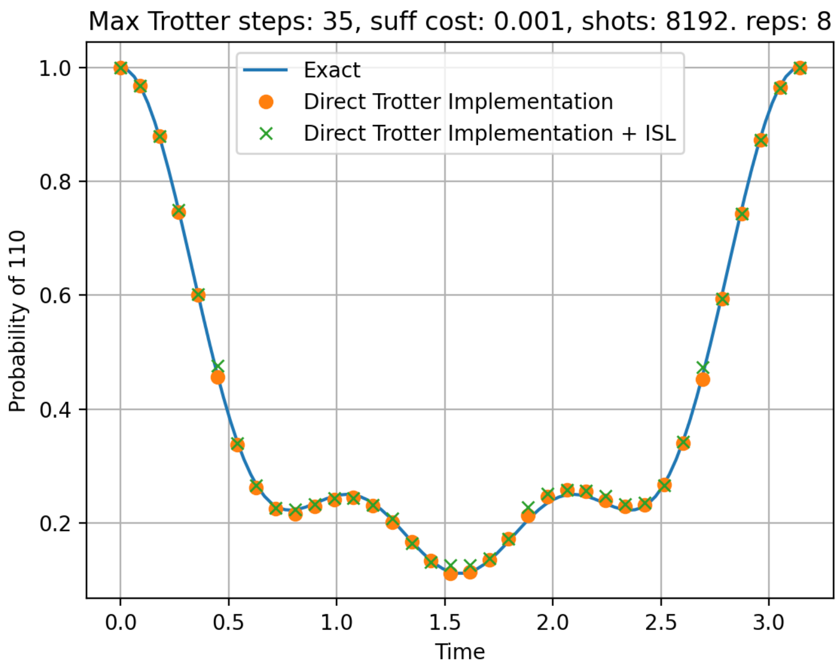

Figure 5: Probability of measuring the $|110\rangle$ computational basis state analytically (blue line), or using a Trotterised circuit decomposition without (orange circles) or with approximate circuit recompilation (green crosses). The Trotterised results are obtained on the statevector simulator and then sampled with $k = 8192$ shots.

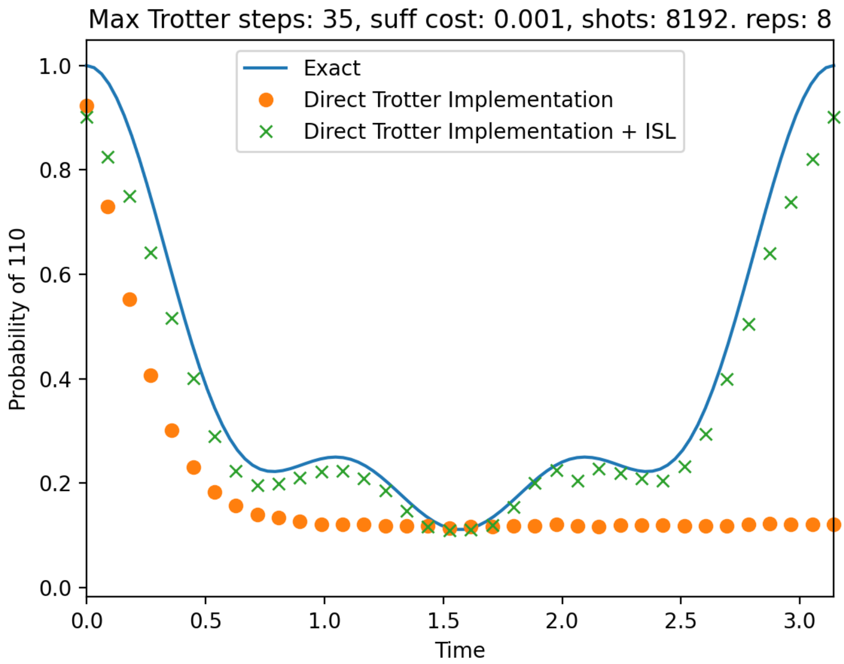

Figure 6: Probability of measuring the $|110\rangle$ computational basis state analytically (blue line), or using a Trotterised circuit decomposition without (orange circles) or with approximate circuit recompilation (green crosses). Here the experiments are evaluated on Fake Jakarta which, which applies a realistic noise profile mimicing the real *ibmq_jakarta*. In the notebook, we reconstruct this graph for different ISL cost values, observing the trade-off between higher accuracy of recompiled solutions and noise generated by more gates. This graph presents the optimum sufficient cost of 0.001.

recompiled circuits once again on the qasm simulator. Here we find that the solutions found by ISL are of high enough quality to allow the exact almost replication of the analytic and non-recompiled dynamics. Importantly, our approximate recompilation routine does not optimise for just the $|110\rangle$ state but for the entire statevector, capturing the rich dynamics of other observables not shown here.

Having established that approximate circuit recompilation with ISL can find solutions that reproduce the desired dynamics, we introduce noise into our circuit evaluations. This will allow us to evaluate whether, despite being able to produce only approximately the correct state, the ISL solutions are shallow enough that the overall noise of the final solution is lower. The answer here is resoundingly yes, as shown in Fig. 6. Firstly, we see that for the non-recompiled solution, the measured probability of the $|110\rangle$ state decays exponentially, plateauing at the uniform random value of $1/2^3$. By contrast, the significantly shallower circuits produced by the ISL algorithm generate far less noise. The result of this is a simulation where the measured probability of the —110¿ is much closer to the form of the analytic solution. Importantly, the number of gates of our recompiled solution does not grow linearly with the simulation time and thus avoids the exponential decay of the observed signal.

Fig. 6 demonstrates the result of another investigation we carry out, namely, what is the optimal sufficient cost for our problem? Whilst a lower sufficient cost will lead to a recompiled circuit which outputs a state much closer to the target state, in general the solution circuit will also contain more gates. These additional gates will in turn produce noise that offsets the theoretical benefit of the higher overlap between the target and recompiled circuits. In the notebook our experiments are presented with a slider, from which we see that the optimal sufficient cost for ISL is 0.001 (as shown here), which we use going forward.

Finally, with the number of Trotter steps required and the optimal sufficient cost found for the given problem and fake *ibmq_jakarta* noise profile, we attempt our ambitious goal of reproducing the entire dynamics on the real device. Fig. 7 shows the result of simulating each of the $n = 1$ to $n = 35$ Trotter step circuits that spans the evolution on the real *ibmq_jakarta* device. Remarkably, our solution combining

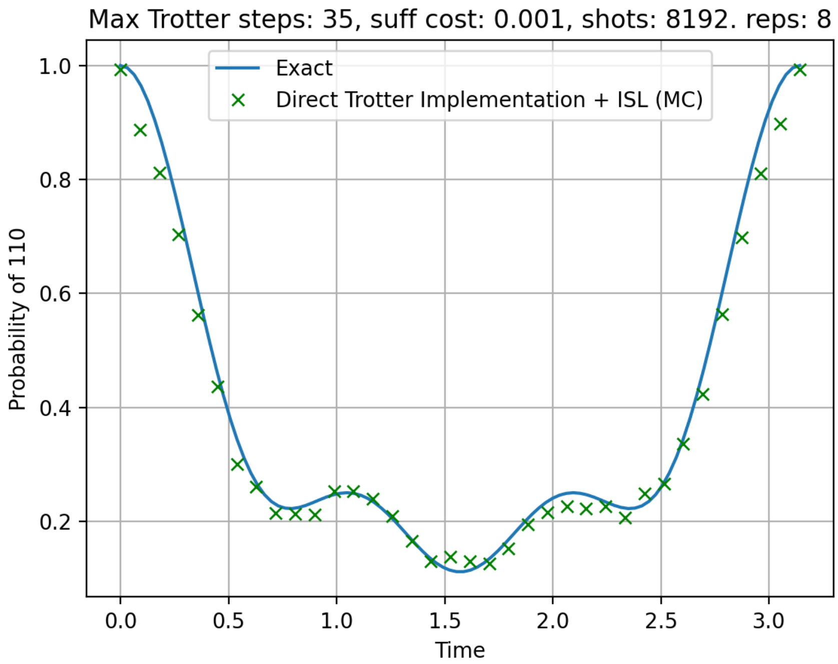

Figure 7: Probability of measuring the $|110\rangle$ computational basis state whilst evolving $|\psi_{\text{init}}\rangle = |110\rangle$ under the XXX Heisenberg spin model, as obtained analytically (blue line) or on the real *ibmq_jakarta* (green crosses). For running on the quantum hardware, device errors are minimised by using ISL to find approximate shallower equivalents of the Trotterised Hamiltonian and applying measurement calibration (MC).

both ISL approximate circuit recompilation and measurement calibration is able to reproduce the form of the analytic solution, calculating the probability of the $|110\rangle$ state within on average 2.4 percentage points of the true value. This constitutes our attempt at achieving the ambitious goal of reproducing the complete dynamics of the XXX Heisenberg spin model on the real device. Whilst some inaccuracies remain, our results clearly demonstrate the interesting physics of the model under study and strongly agree with the analytic solution, retaining its symmetry. Most importantly, by simulating the entire graph on real quantum hardware, we hope to have demonstrated that our solution is general to any amount of evolved time.

Completing our results, we then present a specific case of the above graph which is the benchmark evolution $t = \pi$. An interesting property of this particular point of the evolution, also a consequence of the periodicity of the model, is that the probability of the —110¿ state is 1. This means that ultimately, any accurate circuit reproducing the evolution will prepare the qubits exactly into the —110¿ state. This has important consequences for our approximate recompilation solution. When recompiling the Trotterised solution with low enough Trotter error, the problem for our ISL solver can be thought as ”given a circuit that prepares the —110¿ state, find a set of gates which maps this back to the —000¿ state”. This is perhaps clearer when we restate the ISL cost function $C = 1 - |\langle 0|V^\dagger U|0\rangle|^2$.

The result of this is that the recompiled solution we obtain consists of a single X gate followed by a CNOT, effectively preparing the —110¿ state. Interestingly, this is not the lowest depth possible solution, since the same transformation could be made with just two X gates. However, as described previously, ISL incrementally builds an equivalent circuit with layers of thinly dressed CNOT gates. Whilst this allows the success seen in Fig. 7, producing shallow circuits able to reproduce any part of the dynamics, it means a solution with zero CNOT gates cannot be produced. So in effect, we are not able to obtain the absolute shortest time circuit possible due to our desire for our solution to be general when constructing it.

Running the *ibmq_jakarta* tomography procedure on the recompiled circuit that produces the benchmark evolution $t = \pi$, we obtain a fidelity of 0.993. This marks the end of our submission and our final result.

	Without ISL	With ISL
Without MC	0.119*	0.886
With MC	0.121*	**0.993**

Table 1: Fidelities obtained running the provided tomography routine on the *ibmq_jakarta* device. This compares the quantum state produced by the Trotterised time evolution circuit to the exact $|110\rangle$ state, with and without incremental structural learning and measurement calibration. Values with a * indicate obtained on Fake Jakarta.

Table 1 shows the fidelities obtained in different experiments on *ibmq_jakarta* with and without the two different error mitigation techniques used in our submission.

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