Neural Error Mitigation of Near-Term Quantum Simulations

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Near-term quantum computers provide a promising platform for finding the ground states of quantum systems, which is an essential task in physics, chemistry and materials science. However, near-term approaches are constrained by the effects of noise, as well as the limited resources of near-term quantum hardware. We introduce neural error mitigation, which uses neural networks to improve estimates of ground states and ground-state observables obtained using near-term quantum simulations. To demonstrate our method's broad applicability, we employ neural error mitigation to find the ground states of the H2 and LiH molecular Hamiltonians, as well as the lattice Schwinger model, prepared via the variational quantum eigensolver. Our results show that neural error mitigation improves numerical and experimental variational quantum eigensolver computations to yield low energy errors, high fidelities and accurate estimations of more complex observables such as order parameters and entanglement entropy without requiring additional quantum resources. Furthermore, neural error mitigation is agnostic with respect to the quantum state preparation algorithm used, the quantum hardware it is implemented on and the particular noise channel affecting the experiment, contributing to its versatility as a tool for quantum simulation.

Since the early twentieth century scientists have been developing comprehensive theories that describe the behaviour of quantum mechanical systems. However, the computational cost required to study these systems often exceeds the capabilities of current scientific computing methods and hardware. Consequently, computational infeasibility remains a roadblock for the practical application of these theories to problems of scientific and technological importance.

The simulation of quantum systems on quantum computers, referred to here as quantum simulation, shows promise for overcoming these roadblocks and has been a foundational driving force behind the conception and creation of quantum computers1–4. In particular, quantum simulation of ground and steady states of quantum many-body systems beyond the capabilities of classical computers is expected to substantially impact nuclear physics, particle physics, quantum gravity, condensed matter physics, quantum chemistry and materials science5–9. The capabilities of current and near-term quantum computers continue to be constrained by limitations such as the number of qubits and the effects of noise. 

Quantum error correction techniques can eliminate errors that result from noise, providing a path towards fault-tolerant quantum computation. However, in practice, implementing quantum error correction imposes a large overhead in terms of both the required number of qubits and low error rates, both of which remain beyond the capabilities of current and near-term devices.

Until fault-tolerant quantum simulations can be realized, modern variational algorithms substantially alleviate demands on quantum hardware and exploit the capabilities of noisy intermediate-scale quantum devices10,11. One prominent example is the variational quantum eigensolver (VQE)12, a hybrid quantum–classical algorithm that iteratively approximates the lowest-energy eigenvalues of a target Hamiltonian through the variational optimization of a family of parameterized quantum circuits. This, among other variational algorithms, has emerged as a leading strategy for achieving a quantum advantage using near-term devices and accelerating progress in multiple scientific and technological fields13–15.

The experimental implementation of variational quantum algorithms remains a challenge for many scientific problems, as noisy intermediate-scale quantum devices suffer from various sources of noise and imperfection. Several methods for quantum error mitigation (QEM) to alleviate these issues have been proposed and experimentally validated, improving quantum computations in the absence of the quantum resources required for quantum error correction16. For a review of current QEM techniques, we refer the reader to the work of Endo et al.13 and the literature cited therein. In general, these methods use specific information about the noise channels that affect a quantum computation, the hardware implementation or the quantum algorithms themselves. Examples include the implicit characterization of noise models and how they affect estimates of the desired observables, specific knowledge of the state subspaces in which the prepared quantum state ought to reside and the characterization and mitigation of the sources of noise on individual components of the quantum computation, such as single- and two-qubit gate errors, as well as state preparation and measurement errors.

Machine learning techniques, which have recently been repurposed as tools for tackling complex problems in quantum many-body physics and quantum information processing17,18, provide an alternative route to QEM. Here we introduce a QEM strategy named neural error mitigation (NEM), which uses neural networks to mitigate errors in the approximate preparation of the quantum ground state of a Hamiltonian.

The NEM algorithm, summarized in Fig. 1, is composed of two steps. First, we performed neural quantum state (NQS) tomography (NQST) to train an NQS ansatz to represent the approximate

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ground state prepared by a noisy quantum device using experimentally accessible measurements. Inspired by traditional quantum state tomography (QST), NQST is a data-driven machine learning approach to QST that uses a limited number of measurements to efficiently reconstruct complex quantum states. We then applied the variational Monte Carlo (VMC) algorithm on the same NQS ansatz (which we call the NEM ansatz) to improve the representation of the unknown ground state. In the spirit of the VQE, VMC approximates the ground state of a Hamiltonian on the basis of a classical variational ansatz, in this case an NQS ansatz.

Here we used an autoregressive generative neural network as our NEM ansatz; more specifically, we used the Transformer architecture and show that this model performs well as an NQS. Owing to its capability to model long-range temporal and spatial correlations, this architecture has been used in many state-of-the-art experiments in natural language and image processing and has the potential to model long-range quantum correlations. We refer the reader to the Methods and Supplementary Information for a complete description of NQSs, NQST, VMC, and the Transformer neural network.

NEM has several advantages over other error mitigation techniques. First, it has a low experimental overhead; it requires only a set of simple experimentally feasible measurements to learn the properties of the noisy quantum state prepared by VQE. Consequently, the overhead of error mitigation in NEM is shifted from quantum resources (that is, performing additional quantum experiments and measurements) to classical computing resources for machine learning. In particular, we note that the primary cost of NEM is in performing VMC until convergence. Another advantage of NEM is that it is agnostic with respect to the quantum simulation algorithm, the device it is implemented on and the particular noise channel affecting the quantum simulation. As a result, it can also be combined with other QEM techniques and can be applied to either analogue quantum simulation or digital quantum circuits.

NEM also addresses the low measurement precision that arises when estimating quantum observables using near-term quantum devices. This is particularly important in quantum simulations, where making accurate estimations of quantum observables is essential for practical applications. NEM intrinsically resolves the low measurement precision at each step of the algorithm. During the first step, NQST improves the variance of observable estimates at the cost of introducing a small estimation bias. This bias, as well as the remaining variance, is further reduced by training the NEM ansatz using VMC, which results in a zero-variance expectation value for energy estimates once the ground state has been reached.

**Results**

**Quantum chemistry results.** Accurately simulating a molecule’s electron correlations is an integral step in characterizing the chemical properties of the molecule. This problem, known as the electronic structure problem, involves finding the ground-state wavefunction and energy of many-body interacting fermionic molecular Hamiltonians. Achieving an absolute energy error |ΔE| corresponding to chemical accuracy (1 kcal mol$^{-1}$ ≈ 0.0016 hartrees, the threshold for accurately estimating room-temperature chemical reaction rates) is essential for applications in drug discovery and materials science.

We demonstrate the application of NEM to the estimation of molecular ground states prepared using a VQE algorithm and show that our method improves the results up to chemical accuracy or better for H$_2$ and LiH molecules (see Fig. 2 for experimental and numerical results). We mapped the H$_2$ and LiH molecular Hamiltonians computed in the Slater-type orbital (STO-3G) basis to qubits Hamiltonians with $N=2$ and $N=4$ qubits, respectively. The prepared quantum state was the hardware-efficient variational quantum circuit composed of single-qubit Euler rotation gates and two-qubit controlled NOT entangling gates native to superconducting hardware. For both H$_2$ and LiH, we constructed variational circuits with a single entangling layer, giving variational circuits with 10 and 20 parameters, respectively. More details can be found in the Methods.

We highlight the performance of NEM on the experimental preparation of the ground states of LiH at different bond lengths using IBM’s five-qubit chip, IBMQ-Rome. We mapped the four-qubit LiH problem to the four linearly connected qubits on IBMQ-Rome that had the lowest average single- and two-qubit gate errors. During optimization, we performed 250 iterations of simultaneous perturbation stochastic approximation optimization to obtain the final prepared quantum state. NEM improves the results of VQE to chemical accuracy or better for all bond lengths and achieves infidelities (given by $1-|\langle \Psi | \Psi \rangle|^2$) of $10^{-3}$ for most bond lengths (shown in Fig. 2a–c). On average, NEM achieves an improvement of three orders of magnitude in energy estimation and two orders of magnitude in infidelity. We provide further details about the reconstruction quality in the Supplementary Information, including an analysis of the reconstructed NQS.

We also illustrate the results of applying NEM on the ground states of H$_2$ and LiH prepared using classically simulated VQE with a depolarizing noise channel (shown in Fig. 2d–i). We simulated VQE with a single-qubit depolarizing error probability of 0.001 and two-qubit depolarizing error probability of 0.01. At each bond length, we generated ten VQE simulations and report the NEM results. Notably, the median performance of NEM improves the ground-state estimation of H$_2$ and LiH to chemical accuracy and low infidelities for all bond lengths. The increased infidelity for bond lengths longer than 2 Å, as shown in the infidelity plots of Fig. 2, can be explained by the decreasing energy gap between the ground state and the first excited state. When the energy gap is small, it becomes more difficult for methods that optimize the energy, such as VQE and VMC, to isolate the ground-state representation.

**Lattice Schwinger results.** We next applied our method to the ground state of the lattice Schwinger model, which is a prototypical Abelian lattice gauge theory, and a toy model for quantum electrodynamics in one spatial dimension. Multiple experiments that use quantum devices to explore the properties of this model have been proposed. Here we consider the experiment in which a
Experimental and numerical NEM results for molecular Hamiltonians. a–i, NEM results for energy (a,d,g), $|\Delta E|$ (b,e,h) and infidelity (c,f,i) for the ground states of LiH and $H_2$ prepared using a hardware-efficient variational quantum circuit. a–c, Results for the LiH ground state prepared experimentally using IBMQ-Rome. d–f, The performance of NEM for numerically prepared $H_2$ ground states. g–i, The performance of NEM for numerically prepared LiH ground states. Results are shown for the median performance over ten noisy numerical simulations per bond length, and the shaded region is the interquartile range. For our ten data points, the interquartile range includes the middle six and excludes the best two and worst two to indicate the typical performance of the method. Error mitigated results extend both the experimentally and numerically prepared VQE states to chemical accuracy and low infidelities for all bond lengths of LiH and $H_2$. Chemical accuracy is shown at 0.0016 hartrees (dashed black line).

Trapped-ion analogue quantum simulator is used to variationally prepare the ground state of the lattice Schwinger model using alternating entangling operations, $e^{i H \Delta t}$, which simultaneously act on all qubits with an entangling Hamiltonian $H_2$ for some time $\Delta t$, and single-qubit rotations (shown in Extended Data Fig. 1). After using a Jordan–Wigner transformation to map the fermionic degrees of freedom of the theory to qubits, the lattice Schwinger Hamiltonian takes the following form:

$$H = \frac{w}{2} \sum_{j=1}^{N-1} (\hat{X}_j \hat{X}_{j+1} + \hat{Y}_j \hat{Y}_{j+1}) + \frac{w}{2} \sum_{j=1}^{N} (\hat{Z}_j + \hat{g} \hat{L}_j^2).$$

Here, $\hat{X}, \hat{Y}, \hat{Z}$ and $\hat{I}$ are the Pauli operators and $j$ is a site index. The first term describes the creation and annihilation of electron–positron pairs and contains an overall energy scale, $w$. The second term contains the bare electron mass $m$, and the third term contains $\hat{g}$, which is the coupling strength to the electric field $\hat{L}_j$. Solving for the electric field in one spatial dimension gives

$$\hat{L}_j = \varepsilon_0 - \frac{1}{2} \sum_{\epsilon=1}^{N} \left( \hat{Z}_j + (-1)^j \hat{I} \right)$$

where $\varepsilon_0$ is an integration constant and $j$ is a site index. Given that the quantum fields at one spatial lattice point are encoded into a pair of qubits, the total number of sites $N$ must be even. We set $w = 1$, $\hat{g} = 1$ and $\varepsilon_0 = 0$ such that the only remaining parameter is $m$. The ground state of the system for $m \to +\infty$ describes a vacuum with no electron–positron pairs and that for $m \to -\infty$ describes a large number of electron–positron pairs. In the thermodynamic limit, the model exhibits a second-order phase transition at $m \approx -0.7$, which can be detected using the order parameter

$$\langle O \rangle = \frac{1}{N} \sum_{j=1}^{N} \left( 1 + (-1)^j \hat{Z}_j \right).$$

The model possesses discrete symmetries, which inform the choice of a variational quantum circuit with a manageable number of parameters, but to demonstrate the general applicability of NEM we did not enforce these symmetries on the NQS. We demonstrated the performance of NEM by applying it to the approximate ground state of the lattice Schwinger model obtained by numerically simulating a VQE algorithm for $N=8$ sites, with single-qubit depolarizing noise with probability $\lambda = 0.001$ applied after each rotation and entangling operation. As shown in Fig. 3, the simple VQE scheme we employed exhibits median infidelities between 0.10 and 0.31, with worst performance closer to the phase transition around $m = -0.7$. Although the qualitative behaviour of the ground-state energy as a function of the mass is modelled approximately by VQE, the qualitative behaviour of other physical properties is not reproduced well, limiting the utility of our VQE results for studying the phase transition. This includes the order parameter and the Renyi entanglement entropy $S_\alpha$ of a partition of the system, which is a widely used, experimentally accessible quantity that expresses the amount of correlation present in the quantum state.

The properties of the NEM state showed a substantial improvement over VQE. The NEM state reached absolute energy errors on the order of $10^{-3}$ and infidelities approaching $10^{-5}$. Importantly, after applying NEM, the physical properties estimated by the state accurately followed their exact values. The ability to obtain precise
estimations of these physical properties can be explained by the accurate representation of the ground-state wavefunction captured by the NEM NQS. Further details about the reconstruction quality of each component are covered in the Supplementary Information, including a thorough analysis of the NEM NQSs.

To gather evidence that the performance of NEM scales well to larger near-term experiments on quantum devices, we studied the behaviour of NEM as a function of system size for the lattice Schwinger model. For computational efficiency, the scaling study used a modified VQE implementation without noise (Fig. 3e,f) compared with the simulated trapped-ion experiment (Fig. 3) (see Methods for more details of the modified circuit). The VQE algorithm was simulated on a classical computer for system sizes up to $N = 16$, and NEM was applied to the resulting states. The results in Fig. 3e,f show that NEM improved on the VQE results by two to four orders of magnitude, even when using a small VMC batch size of $b = 2^n$, which is the number of samples used to estimate the energy’s gradient in one iteration of VMC. In all panels, median values over ten runs are shown, and the shaded region is the interquartile range.

By combining VQE, which uses a parametric quantum circuit as an ansatz, and NQST and VMC, which use neural networks as an ansatz, NEM brings together two families of parametric quantum states and three optimization problems over their loss landscapes. Our work raises the question of the nature of the relationships between these families of states, their loss landscapes and quantum advantage. Examining these relationships offers a new way to investigate the potential of noisy intermediate-scale quantum algorithms in seeking a quantum advantage. This may lead to a better delineation between classically tractable simulations of quantum systems and those that require quantum resources.

Methods

**NQS.** Our NQS was based on the Transformer architecture, which was developed to process sequences that have temporal and spatial correlations, such as written languages. Compared with previous architectures for sequence models such as the long short-term memory neural network, the Transformer excels at modelling long-range correlations and has thus become very popular in machine learning. Within the quantum many-body machine learning community there has been a lot of work using autoregressive neural networks as NQSs. Recently, the Transformer has been adapted as an autoregressive generative NQS.

We represent the quantum state $|\psi\rangle$ with a Transformer neural network that takes as input a bitstring $s = (s_1, s_2, \ldots, s_N) \in [0,1]^N$, describing a computational basis state $|s\rangle$, where $N$ is the number of qubits. The neural network outputs two numbers ($p_s(s), q_s(s)$) parameterized by the neural network weights $\lambda$, which form the complex amplitude $a_s|\psi\rangle$ given by

$$a_s = \sqrt{p_s} e^{i q_s}.$$  

Here, $p_s(s)$ is a normalized probability distribution, which automatically normalizes the quantum state. The autoregressive property of the model allows efficient sampling from the Born distribution of $|\psi\rangle$ in the computational basis. More details can be found in the Supplementary Information.

The exact ground-state amplitudes of both the quantum chemistry models and the lattice Schwinger model are real; that is, $q_s(s) \in [0, \pi]$, and the signs of the lattice Schwinger model ground-state amplitudes follow a simple sign rule. However, to show the general applicability of our method, we did not enforce any of these conditions in our NQSs.

**NQST.** In NQST, a neural network is trained to represent the state of a quantum device using samples from that state in various Pauli bases (that is, after
performs various post-rotations). NQST proceeds by iteratively adjusting the NQS parameters to maximize the likelihood that NQS assigns to the samples. A sample $s \in \{0, 1\}^N$ in a Pauli basis $B = \{I, X, Y, Z\}$, with $P_e \in \{X, Y, Z\}$, is the unique simultaneous eigenstate of the single-qubit Pauli operators $P_e$ with eigenvalues determined by the entries of $s$. We denote such a state $|s, B\rangle$. The likelihood of the sample $(s, B)$ according to the NQS $|\psi_p\rangle$ is given by

$$p_s(B) = \left| \langle s | B | \psi_p \rangle \right|^2 = \sum_{t \in \{0, 1\}^N} \sum_{s, B(t) \neq 0} p_{s, B(t)}(t) \langle t | B | \psi_p \rangle.$$

(3)

Here, we sum over the computational basis states $|t\rangle$ that have a non-zero overlap with the given sample $|s, B\rangle$. For a single sample $|s, B\rangle$, the number of $|t\rangle$ is $2^N$, where $K$ is the number of positions $j$ where $P_e \neq Z$. The computational cost of a single iteration of tomography training is therefore proportional to $2^N$. To constrain this computational cost, we used projective measurements in almost-diagonal Pauli bases (that is, Pauli bases $B$ with low numbers of $X$ or $Y$ terms).

To learn the quantum state from a set of measurements $\mathcal{D}$, the objective function minimized during NQST was an approximation of the cross entropy averaged over the set of bases $B$ from which samples were drawn and is given by

$$L_k = -\frac{1}{|\mathcal{D}|} \sum_{B, s \in \mathcal{D}} p_{QUBO}(s, B) \ln p_s(B).$$

(4)

Here, $p_{QUBO}(s, B)$ is the exact unknown likelihood of measuring $|s, B\rangle$ from the VQE state. The cross entropy achieves its minimum in $K$ if $p_{QUBO}(s, B) = p_s(B)$. As commonly done in unsupervised learning, the cross entropy was approximated using the set $\mathcal{D}$ of the measured $|s, B\rangle$, which was further partitioned into training and validation subsets $\mathcal{D}_{TV}$. The loss function used in training was

$$L_k \approx -\frac{1}{|\mathcal{D}_{TV}|} \sum_{s \in \mathcal{D}_{TV}} \ln p_s(B).$$

(5)

The training was performed using stochastic gradient descent with the Adam optimizer.

VMC and regularization. VMC is a method that adjusts the parameters of a classical variational wavefunction ansatz to approximate the ground state of a given Hamiltonian. The method usually proceeds by gradient-based optimization of the energy, where the energy and its partial derivatives with respect to the ansatz parameters are estimated using Monte Carlo samples drawn from the classical variational wavefunction. As detailed in the Supplementary Information, the autoregressive property of our neural network wavefunction allows efficient classical variational wavefunction. As detailed in the Supplementary Information, the variational circuit was then optimized using Qiskit’s implementation of the VQE variational quantum eigensolver code, which allowed exact sampling of the learned probability distribution and was automatically normalized. More details on the regularization term and the VMC algorithm can be found in the Supplementary Information.

The VQE implementation for quantum chemistry. We used the variational quantum circuit in equation (6) for the electronic structure problem in quantum chemistry. This ansatz was designed for the hardware capabilities of current superconducting quantum processors \(^1\). We used this circuit for both our numerical simulations with a depolarizing noise channel and to perform experiments on a five-qubit superconducting quantum processor (Fig. 2).

The $H_2$ and LiH molecular Hamiltonians were mapped to qubit Hamiltonians with $N = 2$ and $N = 4$ qubits, respectively \(^{26}\). Specifically, we mapped the second-quantized fermionic Hamiltonian for $H_2$ to its qubit Hamiltonian using the Bravyi–Kitaev transformation \(^{25}\) while the LiH Hamiltonian was transformed using the parity transformation \(^{40}\). In each case, two qubits associated with the spin–parity symmetries of the model were removed to obtain final qubit Hamiltonians \(^{41}\).

The hardware-efficient variational quantum circuit was composed of single-qubit rotations and two-qubit entangling gates native to superconducting hardware. The variational circuit, for $N$ qubits consisting of $d$ controlled NOT entangling (ENT) layers alternating with $N/(d + 1)$ single-qubit Euler (EUR) rotation. Each Euler rotation

$$U_{EUR}(\theta) = R_z(\theta) R_x(\theta) R_z(\theta),$$

was composed of three single-qubit rotation gates $R(\theta)$ parameterized by an angle $\theta$. In the first rotation layer, $U^{d+1}(\theta)$, the first set of $Z$ rotations was not implemented, reducing the number of circuit parameters. Within each entangling layer, we applied controlled NOT gates on pairs of linearly connected qubits. The variational circuit had $p = (N + 2)$ independent parameters. For both $H_2$ and LiH, we constructed a variational circuit with $d = 1$ entangling layers giving 10 and 20 parameters, respectively.

The variational circuit was then optimized using Qiskit’s implementation of simultaneous perturbation stochastic approximation (SPSA)\(^{33}\) for 250 iterations to obtain an estimation for the ground-state energy of $H_2$ and LiH. Each SPSA iteration required two energy evaluations. To reduce the sampling overhead during the energy estimations, Pauli terms in each Hamiltonian were grouped according to their common tensor product basis \(^{29}\), requiring only 2 and 25 circuits with unique post-rotations for $H_2$ and LiH, respectively, to estimate the energy.

To perform NQST, we collected almost-diagonal measurement samples from the variational circuit implemented on the noisy quantum simulator. The Qiskit’s SPSA was followed by the variational procedure. In this case, the nearly diagonal samples were taken in the following bases: in the all-Z basis, in the $X$ and $Z$ diagonal, and in the $N(M-1)/2$ bases with two $X$ and $Z$ diagonal.

The VQE implementation for the lattice Schwinger model. Our variational quantum circuit for the lattice Schwinger model closely followed the variational circuit implementation on a trapped-ion analogue quantum simulator \(^2\) that approximately preserved the symmetries of the lattice Schwinger model. The quantum system was first prepared in $|0\ldots 0\rangle$ for $m \geq -0.7$ and $|10\ldots 10\rangle$ for $m < -0.7$, coinciding with the ground states of the Schwinger Hamiltonian \(^{11}\) for $m = \pm \infty$. On this initial state, three alternating layers of evolution with an entangling Hamiltonian followed by $Z$ rotation each qubit, were applied. The entangling Hamiltonian contained long-range $XY$ couplings and a uniform effective magnetic field and was given by

$$H_2 = \sum_{j=1}^N \sum_{k=1}^N \frac{1}{|j-k|} X_j X_k + B \sum_{j=1}^N Z_j.$$  

(7)

We chose $a = 1, j = 1$ and $B = 0.1$ to approximate the trapped-ion experimental setup \(^9\). Evolution with this Hamiltonian preserved the symmetries of the lattice Schwinger model to first-order terms in $1/B$.

Only half of the particles in each single-qubit rotation layer were independent, as required by the symmetries, giving $g_j = -g_{J-j}$, for $j \in \{N/2+1, \ldots, N\}$. In total, the variational circuit had 15 independent parameters for $N = 8$ lattice sites, which were initialized at zero at the start of each optimization. As a simple noise model, after each entangling layer and each single-qubit rotation layer, a depolarizing channel with $\lambda = 0.001$ was applied to each qubit (Extended Data Fig. 1a).

To optimize the variational parameters, the energy was estimated by taking samples in each of the three tensor product bases $X$, $Y$, and $Z$. The hyperparameters values were chosen by inspecting the variance and approximate gradient at the beginning of the optimization \(^{40}\). The exact values are listed in the Supplementary Information.

As input to NQST, the quantum circuit was taken in each of the following 2N−1 Pauli bases: the all-Z basis, the $(N−1)$ bases with XX at a pair of neighbouring sites (with Z elsewhere) and the $(N−1)$ bases with YY at a pair of neighbouring sites (with Z elsewhere). Note that for the Hamiltonian given by equation (1), the samples provided an estimation of the energy.
The scaling study shown in Fig. 3e,f used a modified VQE implementation for computational efficiency. Instead of evolving the circuit using the entangling Hamiltonian, we used an entangling layer \( \mathcal{C}_2 \) comprising two layers of two-qubit gates simulated without noise, as depicted in Extended Data Fig. 1b. The entangling layer was chosen to exactly preserve the symmetries of the lattice Schrödinger model, while being easier to simulate numerically than evolution with \( \mathcal{H}_2 \). Note that as it was composed of nearest-neighbour gates, it is also suited to superconducting quantum hardware, especially to capacitively coupled flux-tunable transmon devices, in which the interaction \( XX+YY \) is easily implemented\(^{30}\). For the scaling study, 1,024 samples were taken in each basis to estimate the energy during SPSA optimization. The hyperparameter \( \alpha \) of SPSA was increased to 20 and the parameters \( \alpha_2 \) remained unchanged.

### Data availability

The experimental and numerical quantum simulation measurement data shown in Fig. 2 for \( \mathcal{H}_2 \) and \( \mathcal{L} \) and, as well as the measurement data used in Fig. 3a–d for the eight-site lattice Schrödinger model, are available at https://github.com/1QB-Information-Technologies/NEM (see Zenodo repository\(^{50}\)).

### Code availability

The numerical implementation of the NEM and the code used to numerically implement the quantum simulations studied here are available at https://github.com/1QB-Information-Technologies/NEM (see Zenodo repository\(^{50}\)).

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**Author contributions**
E.R.B. and F.H. developed the codebase for all studies, performed numerical experiments and analysed the results. E.R.B. performed experiments using the IBM quantum processor. E.R.B. and F.H. focused on the quantum chemistry and the lattice Schwinger model case studies, respectively. All authors contributed to ideation and dissemination. J.C. and P.R. contributed to the theoretical foundations and design of the method.

**Competing interests**
The authors declare no competing interests.

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Extended Data Fig. 1 | VQE ansatz circuits for the lattice Schwinger model. a, Variational quantum circuit used to prepare the approximate ground state of the lattice Schwinger model, using VQE simulated classically. The input state $|\Psi_0\rangle$ is $|01\cdots01\rangle \langle 10\cdots10\rangle$ for $m \geq -0.7$ ($m < -0.7$). b, For the results shown in Fig. 3e,f, the entangling layers of (a) are replaced with $O_N$ for $N$ sites. The layers of single-qubit gates are left unchanged.