

Programming Optical-Lattice Fermi-Hubbard Quantum Simulators

Cristian Tabares^{1,*} Christian Kokail^{2,3} Peter Zoller^{4,5} Daniel González-Cuadra^{1,3,4,5,†} and Alejandro González-Tudela^{1,‡}

¹*Institute of Fundamental Physics IFF-CSIC, Calle Serrano 113b, 28006 Madrid, Spain*

²*ITAMP, Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts 02138, USA*

³*Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA*

⁴*Institute for Theoretical Physics, University of Innsbruck, 6020 Innsbruck, Austria*

⁵*Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences, 6020 Innsbruck, Austria*

 (Received 19 February 2025; revised 29 May 2025; accepted 21 July 2025; published 19 September 2025)

Fermionic atoms in optical lattices provide a native implementation of Fermi-Hubbard (FH) models that can be used as analog quantum simulators of many-body fermionic systems. Recent experimental advances include the time-dependent local control of chemical potentials and tunnelings, and thus enable us to operate this platform digitally as a programmable quantum simulator. Here, we explore these opportunities and develop ground-state preparation algorithms for different fermionic models, based on the ability to implement both single-particle and many-body high-fidelity fermionic gates, as provided by the native FH Hamiltonian. In particular, we first design variational precompiled quantum circuits to prepare the ground state of the natively implemented FH model, with significant speedups relative to competing adiabatic protocols. Besides, the versatility of this variational approach enables us to target extended FH models, i.e., including terms that are not natively realized on the platform. As an illustration, we include next-nearest-neighbor tunnelings at finite dopings, relevant in the context of d -wave superconductivity. Furthermore, we discuss how to approximate the imaginary-time evolution using variational fermionic circuits, both as an alternative state-preparation strategy and as a subroutine for the quantum Lanczos algorithm to further improve the energy estimation. We benchmark our protocols for ladder geometries, though they can be readily applied to two-dimensional experimental setups to address regimes beyond the capabilities of current classical methods. These results pave the way for more efficient and comprehensive explorations of relevant many-body phases with existing programmable fermionic quantum simulators.

DOI: [10.1103/3nx4-bnyy](https://doi.org/10.1103/3nx4-bnyy)

I. INTRODUCTION

Ultracold atoms in optical lattices are now established as one of the leading platforms to simulate quantum many-body physics [1–4]. The use of fermionic atoms, in particular, has enabled the study of strongly correlated fermionic problems in condensed-matter [5–19] and high-energy physics [20–22]. Traditionally, cold-atom quantum simulators operate in an analog mode, where the system evolves globally under the local Fermi-Hubbard (FH)

Hamiltonian, consisting of nearest-neighbor (NN) tunneling terms and on-site Hubbard interactions. This analog approach complements current efforts on digital simulation with qubit-based devices [23–30], with the advantage of avoiding the overheads of fermion-to-qubit mappings [31–37], as well as showing good performance against errors in the absence of quantum error correction [38–43] and having the capabilities to generate large-scale entanglement [44–47]. In certain regimes, however, ground-state preparation with fermionic cold-atom simulators presents open challenges. This is the case when the energy gap is small and where state preparation is limited by temperature effects and finite coherence times, as well as for models beyond the natively implemented local FH Hamiltonian. Addressing both of these issues is required to observe certain phenomena, such as d -wave superconductivity [48], which is now believed to appear in the presence of next-nearest-neighbor (NNN) tunneling terms [49,50].

*Contact author: cristian.tabares@csic.es

†Contact author: dgonzalezcuadra@fas.harvard.edu

‡Contact author: a.gonzalez.tudela@csic.es

Published by the American Physical Society under the terms of the [Creative Commons Attribution 4.0 International](https://creativecommons.org/licenses/by/4.0/) license. Further distribution of this work must maintain attribution to the author(s) and the published article's title, journal citation, and DOI.

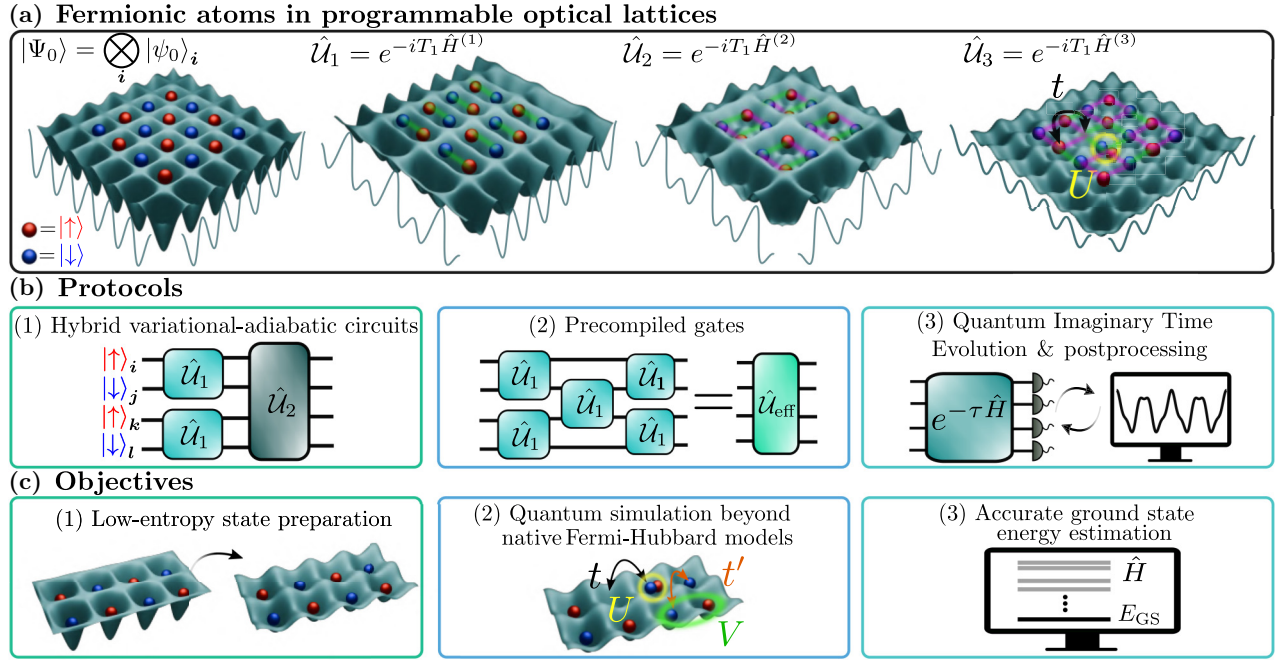


FIG. 1. A schematic illustration of the programmable fermionic quantum simulator architecture introduced in this work. (a) We consider a fermionic quantum processor based on ultracold (spinful) fermionic atoms on a two-dimensional (2D) optical superlattice. The superlattice structure is generated using two counterpropagating laser beams in each direction, giving rise to a four-site unit-cell structure. Our protocols start by first preparing a Mott-insulating state, $|\Psi_0\rangle$, with atoms localized on the potential wells. In the left panel, we represent a half-filled state, but states with finite dopings can also be prepared. In this setup, different unitary gates $\hat{U}_k \in \mathcal{G}$ [see Eq. (5)] can be implemented by globally controlling the superlattice potential. Here, the atoms evolve under the FH Hamiltonian with tunnelings restricted to certain links, as schematically depicted in the other panels. (b) Different protocols built using these resources, and (c) applications in quantum simulation that we target in this work. (1) We construct hybrid variational-adiabatic circuits using sequences of programmable quenched evolutions, allowing us to prepare the ground state of different fermionic Hamiltonians starting from low-entropy product states. (2) Our protocols can be also applied to extended FH models using only the resources depicted in (a), i.e., from the native (local) FH dynamics. To achieve this, we either use the latter to construct precompiled gates that implement unitary evolutions under the extended terms or incorporate their effect through classical postprocessing. (3) The prepared states can be used as inputs to implement a quantum imaginary-time evolution (QITE) and also to improve the estimation of the ground-state energy using the quantum Lanczos (QLanczos) algorithm through classical postprocessing.

Recent experimental advances, including the single-site control and measurement of tunneling elements and chemical potentials using digital mirror devices, optical tweezers, and superlattices [44,51–57], are enabling a more *programmable* mode of operation, allowing us to implement FH dynamics acting only on certain parts of the system. In this context, fermionic atoms in optical lattices can be regarded as *fermionic quantum processors* [58–63], i.e., digital quantum simulators with fermions as their basic constituents. The native dynamics of the system are harnessed here as *resources* to build a set of fermionic gates, which are then used to construct quantum simulation circuits. This approach combines the error resilience of analog devices, since complicated many-body gates can be implemented directly with high fidelity, while incorporating the versatility of digital systems. The latter enables us to prepare ground states more efficiently than traditional adiabatic protocols and to *target* more complicated Hamiltonians that are never directly implemented in

the system. While this programmable approach has been considered for trapped ions [64–66] and Rydberg-atom arrays [67–78], the qubit-based algorithms developed for these platforms cannot be applied directly to cold-atom simulators based on itinerant particles due to the fundamental differences in the hardware architecture and slower experimental repetition rates.

In this work, we focus on the problem of ground-state preparation for extended FH models relevant in condensed-matter physics, including NNN-tunneling terms and NN interactions, and develop protocols especially tailored to the experimental capabilities of fermionic atoms in programmable optical lattices. For this, we first show how to implement a set of fermionic many-body gates generated by FH dynamics [Fig. 1(a)]. While not being universal, this gate set enables the construction of a broad class of state-preparation variational circuits [79] [Fig. 1(b)]. In contrast to previous variational approaches applied to quantum chemistry problems using qubit-based

devices [80–85], the fermionic nature of our resources combined with the translational invariance of the target models allows us to construct circuits with few variational parameters and to considerably reduce or even eliminate costly quantum-classical optimization loops.

The first class of fermionic circuits that we consider can be regarded as *hybrid variational-adiabatic* circuits. Specifically, here the variational part is precompiled classically to prepare the ground state on small system sizes, which are then adiabatically coupled to reach the ground state of the target extended system. This allows us to build finite correlation lengths much faster than purely adiabatic protocols and at the same time avoid any quantum optimization on the hardware.

The second class of variational circuits is inspired by the *quantum imaginary-time evolution* (QITE) [86–89] and can be interpreted as its unitary approximation. While in this case the optimization of the circuit is performed on the quantum hardware, we design our protocols to minimize experimental overheads. In particular, we investigate the effect of shot noise and show that the number of experimental runs required to implement this algorithm is within reach for current cold-atom experiments. Finally, we show that this protocol has the additional advantage that the collected data can be postprocessed using the *quantum Lanczos* (QLanczos) method [86], allowing us to further improve the estimation of the target ground-state energy.

The rest of the paper is structured as follows. We start in Sec. II by introducing a programmable quantum simulator based on fermionic atoms in optical lattices, including the fermionic gate set that can be implemented using the native dynamics of the system. In Sec. III, we build hybrid variational-adiabatic circuits for ground-state preparation using this gate set and apply them to local and extended FH models, both at half filling as well as for finite dopings. In Sec. IV, we explain how to implement QITE using fermionic circuits and apply it to approximate the ground state of the FH models, as well as to improve the estimation of the ground-state energy through the QLanczos algorithm. Finally, in Sec. V, we summarize our findings and point to future directions.

II. PROGRAMMABLE FERMIONIC QUANTUM SIMULATOR

A. Resource Hamiltonians and fermionic gate set

In this work, we consider a fermionic quantum processor based on fermionic atoms trapped in optical lattice potentials, with two internal levels that codify the spin degree of freedom, $\sigma \in \{\uparrow, \downarrow\}$ [see Fig. 1(a)]. Assuming an optical lattice generated by counterpropagating laser beams, the dynamics of the atomic system can be described by the *resource* local FH Hamiltonian,

$$\hat{H}_{\text{FH}} = \hat{H}_t + \hat{H}_U + \hat{H}_n, \quad (1)$$

consisting of NN-tunneling terms,

$$\hat{H}_t = - \sum_{\langle i,j \rangle, \sigma} t_{i,j} \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma}, \quad (2)$$

on-site Hubbard interactions,

$$\hat{H}_U = U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow}, \quad (3)$$

and local chemical potentials,

$$\hat{H}_n = \sum_{i,\sigma} \mu_{i,\sigma} \hat{n}_{i,\sigma}. \quad (4)$$

Here, $c_{i,\sigma}^{(\dagger)}$ denote the (creation) annihilation fermionic operators corresponding to the σ spin component at the site i of a two-dimensional (2D) square lattice and $\hat{n}_{i,\sigma} = \hat{c}_{i,\sigma}^\dagger \hat{c}_{i,\sigma}$ is the atomic occupation number.

To construct fermionic quantum simulation circuits, we employ a set of unitary gates $\mathcal{G}$ generated by the native FH dynamics,

$$\mathcal{G} = \left\{ e^{-i[\hat{H}_t(t_{i,j}) + H_U(U) + H_n(\mu_i)]T} \right\}_{t_{i,j}, U, \mu_i}. \quad (5)$$

In this work, we consider translational-invariant patterns for $t_{i,j}$ and μ_i [see Fig. 1(a)], implemented through superlattice potentials [54,55,57] and local energy shifts [90–93], respectively, where the latter can be made site and spin dependent by introducing vector light shifts. Together with a homogeneous Hubbard parameter U tuned with Feshbach resonances, this gate set $\mathcal{G}$ can thus be implemented using only global experimental knobs. We will assume that we can turn their corresponding parameters on and off freely, and apply quench evolutions under the corresponding terms, which is what we label as programmable operation.

We note that implementing these many-body fermionic gates using digital qubit devices would require long circuits, the depths of which are limited in the absence of error correction, while here they are realized with high fidelity using the native dynamics of the fermions. Despite not being universal, below we show how this restricted gate set is sufficient to construct different quantum state-preparation protocols for several translational-invariant fermionic Hamiltonians relevant in condensed-matter physics.

B. Initialization and state preparation

For cold atoms in optical lattices acting as analog quantum simulators, the ground state of the FH Hamiltonian given in Eq. (1) can be prepared in the system using different approaches. The standard technique consists on

first cooling down an atomic gas to ultracold temperatures and then adiabatically ramping up the optical lattice, an approach that is limited by the temperatures that can be reached experimentally. Alternatively, one can take a more algorithmic approach by first preparing a low-entropy product state of fermionic atoms,

$$|\Psi_0\rangle = \bigotimes_i |\psi_0\rangle_i, \quad (6)$$

where $|\psi_0\rangle \in \{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}$ denotes the fermionic occupation on each lattice site. In particular, both the half-filled case, with $\rho = 1/L \sum_{i,\sigma} \langle \hat{n}_{i,\sigma} \rangle = 1$, where N is the number of lattice sites, as well as finite dopings, with $\delta = 1 - \rho \neq 0$, can be prepared using pattern-loading techniques [94–97], as has been demonstrated experimentally [44,51,53,54,98]. Besides the Mott-insulator product state, one could also prepare a band-insulator product state [98], which is also the natural starting state used in optical-tweezer arrays [92,99]. Both product states can be adiabatically modified to prepare uncoupled dimers [98,100] and then adiabatically connected to the target state [53,54,92,100–104]. Although this approach is guaranteed to work if the ground state is gapped, it is limited by the coherence time of cold-atom experiments if the gap is small, which is the case for doped phases. Moreover, this approach cannot be applied to target extended FH models, the interactions or tunnelings of which are not natively implemented in the system.

In the rest of the paper, we introduce different state-preparation protocols that address these open questions. We follow the algorithmic approach mentioned above, starting from low-entropy product states given in Eq. (6) that we take as a fermionic computational basis, but instead use variational circuits built from the fermionic gates in $\mathcal{G}$ [see Eq. (5)] to prepare the target ground state [see Fig. 1(b)]. This allows us to reach low entropies with a much shorter implementation time, as well as to target Hamiltonians with extended terms not included in the resource Hamiltonian (see, e.g., Appendix A). As we explain in detail in the following sections, we design these variational algorithms to minimize the corresponding measurement overhead, tailoring them to the measurement capabilities of cold-atom quantum hardware, which we describe in Appendix C.

III. HYBRID VARIATIONAL-ADIABATIC FERMIONIC CIRCUITS

In this section, we design variational fermionic circuits with the resources described in Sec. II to approximate the ground states of relevant condensed-matter Hamiltonians. To illustrate the power of these variational circuits, we consider first the local FH model $\hat{H}_{\text{FH}}$ on a ladder geometry and target a strongly correlated regime with $U/t = 8$, both

at half filling (Sec. III A) and finite dopings (Sec. III B). In Sec. III C, we show how these protocols can be also applied to extended FH models.

A. Fermi-Hubbard ladders at half filling

The first target Hamiltonian is the local FH model given in Eq. (1), with $t_{i,j} = t$ and $\mu_i = 0$. This model has been regarded as a candidate to explain high- T_c superconductivity in cuprate materials [48], although recent numerical evidence suggests that it does not support a dominant superconducting order in the expected parameter regime [49]. Nevertheless, the local FH model features other interesting strongly correlated phases, such as stripe phases [12], away from half filling.

As an initial state for our protocol, we consider an anti-ferromagnetic product state $|\Psi_0\rangle$ on a ladder geometry [see Fig. 2(a)]. This state is the half-filled ground state of the Hamiltonian

$$\hat{H}^{(0)} = -\mu \sum_i (-1)^{i_x+i_y} (\hat{n}_{i,\uparrow} - \hat{n}_{i,\downarrow}), \quad (7)$$

where $\mathbf{i} = (i_x, i_y)$. The steps of the protocol are schematically depicted in Figs. 2(b)–2(d): (i) we first prepare the ground state of $\hat{H}_{\text{FH}}$ for a product of uncoupled dimers; (ii) we then couple neighboring dimers to obtain the ground state of 2×2 plaquettes; and, finally, (iii) we obtain the ground states of $\hat{H}_{\text{FH}}$ for the whole system by coupling neighboring plaquettes. Each step k of the protocol can be described as a variational quantum circuit consisting of a sequence of global unitary evolutions from our fermionic gate set $\mathcal{G}$ [see Eq. (5)],

$$\hat{\mathcal{U}}^{(k)}(\boldsymbol{\theta}^{(k)}) = \prod_{\mu=1}^{D^{(k)}} e^{-iT_{\mu}^{(k)} \hat{H}_{\mu}^{(k)}(\boldsymbol{\lambda}_{\mu}^{(k)})}. \quad (8)$$

Here, $D^{(k)}$ denotes the depth of the circuit for each step k , $\boldsymbol{\theta}^{(k)} = (\boldsymbol{\theta}_1^{(k)}, \dots, \boldsymbol{\theta}_D^{(k)})$ are variational parameters and $\hat{H}^{(k)}$ are the programmable FH Hamiltonians depicted in Fig. 2 and written explicitly in Appendix B. For each step, we keep certain Hamiltonian couplings fixed and use other ones, denoted by the vector $\boldsymbol{\lambda}_{\mu}^{(k)}$, together with the evolution times $T_{\mu}^{(k)}$, as variational parameters $\boldsymbol{\theta}_{\mu}^{(k)} = T_{\mu}^{(k)} \boldsymbol{\lambda}_{\mu}^{(k)}$. The latter are optimized to minimize the expectation value of the target Hamiltonian over the prepared state using the variational quantum eigensolver (VQE) algorithm [79].

In the following, we use as figures of merit to benchmark the protocols both the residual energy ε and the infidelity $\mathcal{I}$, defined as

$$\varepsilon = \frac{|E(\boldsymbol{\theta}^{(k)}) - E_{\text{GS}}|}{N}, \quad (9)$$

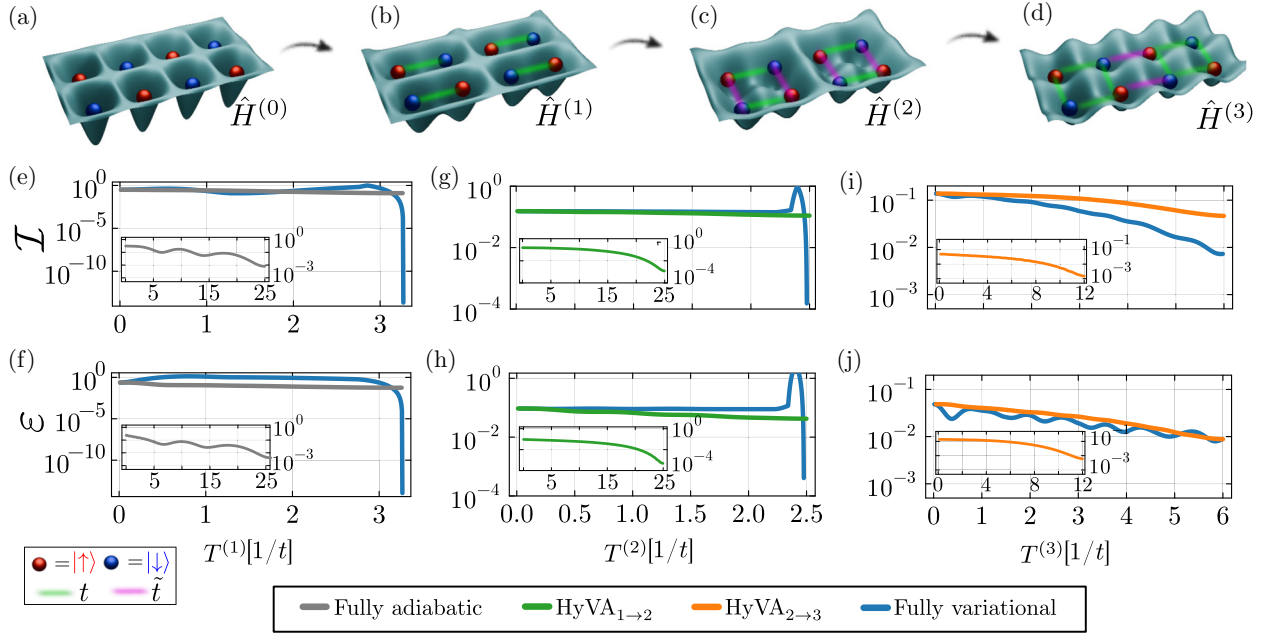


FIG. 2. Ground-state preparation for the local FH model at half filling. (a)–(d) Superlattice configurations employed to prepare the ground state of the local FH model on a 2×4 ladder at half filling and for $U/t = 8$, starting from an antiferromagnetic product state on a deep lattice (a). We employ quench evolutions under the corresponding Hamiltonians $\hat{H}^{(k)}$, where we depict the different nonzero tunneling elements in different colors. We first prepare the ground state on each uncoupled dimer (b), then for each uncoupled plaquettes (c), and finally for the full extended system (d). (e),(g) The infidelity $\mathcal{I}$ and the residual energy ε , respectively, as a function of the implementation time $T^{(1)}$ to prepare a product of uncoupled dimers (b) from the initial product state in (a), using both variational and adiabatic protocols. The inset shows the results obtained with a longer adiabatic protocol. (g),(h) $\mathcal{I}$ and ε as a function of $T^{(2)}$ during the preparation of the ground state for a product of uncoupled plaquettes (c). Both protocols start from the state prepared variationally in (b) and $\text{HyVA}_{1 \rightarrow 2}$ corresponds here to the adiabatic evolution of the latter to the target state. In the inset, we show results obtained for a longer adiabatic evolution. (i),(j) $\mathcal{I}$ and ε for the preparation of the ground state of the target Hamiltonian, i.e., the local FH model (d), as a function of $T^{(3)}$, starting from the state prepared in (c). In this case, the adiabatic part in the $\text{HyVA}_{2 \rightarrow 3}$ protocol refers only to the adiabatic fusion of the uncoupled plaquettes, which are prepared with the fully variational protocol in (c). In the inset, we again show the results obtained after applying the HyVA protocol for longer times.

$$\mathcal{I} = 1 - \mathcal{F}, \quad (10)$$

where $E(\boldsymbol{\theta}^{(k)}) = \langle \psi(\boldsymbol{\theta}^{(k)}) | \hat{H}_{\text{FH}} | \psi(\boldsymbol{\theta}^{(k)}) \rangle$ is the expectation value of $\hat{H}_{\text{FH}}$ over the variational state after each step $|\psi(\boldsymbol{\theta}^{(k)})\rangle = \hat{U}^{(k)}(\boldsymbol{\theta}^{(k)}) |\psi(\boldsymbol{\theta}^{(k-1)})\rangle$, E_{GS} is the exact ground-state energy, and $\mathcal{F} = |\langle \psi_{\text{GS}} | \psi(\boldsymbol{\theta}^{(k)}) \rangle|$ is the fidelity between the variational and the exact ground state $|\psi_{\text{GS}}\rangle$. We note that $E(\boldsymbol{\theta}^{(k)})$ can be measured experimentally using quantum gas microscopes [105–108], as we explain in Appendix C.

As we describe now in detail, in the first two steps a short circuit will be sufficient given the small system size of the target states, and we can thus optimize the circuit classically and apply the resulting optimal evolution directly on the quantum hardware. We refer to these variational circuits as variational *precompiled*, to distinguish them from the ones required in step (iii), where the optimization should be performed on the quantum hardware or replaced by an adiabatic fusion.

In Figs. 2(e) and 2(f), we show the results for the first step of the protocol, where we prepare a product of dimers. We compare the results obtained for an optimized variational circuit with $D^{(1)} = 3$ with an adiabatic fusion of the dimers, and plot the evolution of ε and $\mathcal{I}$ up to the total evolution time, $T^{(1)} = \sum_{\mu} T_{\mu}^{(1)}$. We note that the finite-depth variational circuit prepares *exactly* the ground state of the FH Hamiltonian on each uncoupled dimer. Compared to this, an adiabatic protocol interpolating from $\hat{H}^{(0)}$ to $\hat{H}_{\text{FH}}$ using the same implementation time does not reach similar accuracies, one fifth of the total time being used to ramp up the values of t and U from zero and the rest used to decrease μ . As shown in the inset, by increasing the adiabatic implementation time to $T = 25/t$, the resulting state is still limited to $\mathcal{I} \sim 10^{-2}$ and $\varepsilon \sim 10^{-3}$. We thus conclude that the precompiled variational circuit prepares the state with a much higher accuracy, requiring, moreover, a much shorter implementation time.

The results obtained for the second step of the protocol are shown in Figs. 2(g) and 2(h), where we prepare the ground state of a product of uncoupled plaquettes

starting from the dimer product state, again taking $D^{(2)} = 3$. We now compare these results with those obtained using a hybrid protocol, where we start from the same state but then implement an adiabatic linear ramp of $\tilde{t}$ from 0 to t . We refer to this as a hybrid-variational adiabatic (HyVA_{1→2}) approach. In this case, the fully variational protocol provides much better results, as it prepares the ground state of the uncoupled plaquettes with $\mathcal{I} \sim 10^{-4}$, and with an implementation time 10 times shorter. Moreover, the sudden increase in the figures of merit followed by a fast decay suggests that the variational coupling can be understood as a nonadiabatic process [77].

In the final step, we switch on the tunneling elements between different plaquettes to prepare the ground state of the complete 2×4 ladder [see Fig. 2(d)]. In this case, we use the intraplaquette tunnelings $\tilde{t}_\mu$ and the total evolution time for each quench T_μ as variational parameters. In Figs. 2(i) and 2(j), we show the results for a circuit with $D^{(3)} = 3$ quench evolutions, where we obtain a fidelity above 99.9%. We compare these results with those obtained using a HyVA_{2→3} protocol, starting now from the same variationally prepared plaquettes, which are then adiabatically fused using a linear ramp for the plaquette coupling. In this case, the fully variational protocols require half of the implementation time compared to the HyVA protocol to reach the same fidelities. Moreover, as we discuss in Appendix D, the variational protocols have a certain resilience to noise in the parameters. There, we show that the advantage of these protocols holds even in the presence of experimentally available fidelities.

These results show that even if the HyVA_{2→3} protocol is a bit slower, the difference is not very large compared to the fully variational one. Moreover, the former has the additional advantage that it only relies on precompiled variational circuits to prepare the ground state of the uncoupled plaquettes, which can be optimized classically, as we show in the second step. Thus, it can be implemented directly on the quantum hardware for an extended 2D system, as opposed to a fully variational method. The latter requires a quantum-classical optimization loop [79], which is challenging to implement in cold-atom setups due to current experimental repetition rates [109,110]. Considering these numbers, we estimate that around 300–500 energy evaluations can be implemented in practice [111]. Using a gradient-free optimizer, this means that it would be reasonable to run between three and five hybrid quantum-classical optimization loops with current experimental repetition rates (greater system sizes could be achieved following these variational state preparations with HyVA coupling). We also want to note that the good performance of the HyVA_{2→3} protocol relies on the finite correlation length of the target ground state and it is reminiscent of a renormalization-group approach. The precompiled variational circuits efficiently build up such correlations on plaquettes using a much shorter evolution

time than their adiabatic counterparts, such that the final ground state can be then efficiently prepared by adiabatically coupling them. Since the building blocks of these adiabatic equivalents have been theoretically analyzed previously [101–103] and have already been demonstrated experimentally [53,54,98,100], we expect our ideas to be realizable with current technology. In the following, we drop the subindices and refer to this last protocol as HyVA.

Let us also note that from the behavior shown in Fig. 2 when coupling the smaller to the larger systems, we expect a favorable scaling of our protocols with system size. Due to translational invariance, the coupled subsystems will resemble the final system more as more steps are implemented. Furthermore, since the subsystems are coupled through evolution in time in a Floquet-like scheme, we expect the generated states to accurately match the properties of the target states even in cases in which long-range correlations are involved or small gaps would be crossed [112–114], provided that enough coherence time is available. In the next section, we investigate the performance of this protocol for a different system size, showing that the advantage is still maintained for larger systems.

We finish this section by computing different observables in the states prepared with the hybrid and the fully variational protocols. In Fig. 3, we plot different correlation functions, which can be measured in cold-atom experiments using state-of-the-art techniques, such as quantum gas microscopes [105–107]. In particular, in Fig. 3(a) we show the spin-spin correlations $\langle \hat{S}_i^z \hat{S}_j^z \rangle$ between the atoms within one plaquette. We observe how the HyVA_{1→2} protocol does not manage to build the antiferromagnetic correlations present in the exact ground state, as opposed to the fully variational circuit for the same evolution time. In

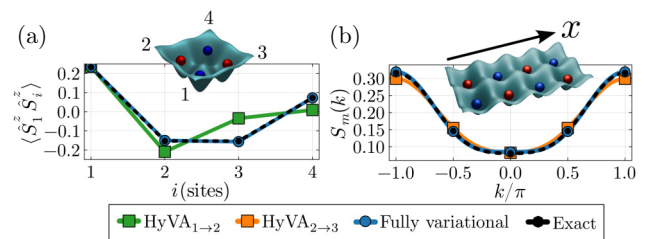


FIG. 3. Observables for the prepared states. (a) Spin-spin correlations between the atoms forming one (uncoupled) plaquette, measured on the state prepared after the second step of our protocol [see Fig. 2(c)]. We compare the results with the fully variational circuit (in blue) and the HyVA_{1→2} approach (in orange) with the same total implementation time. (b) The spin-structure factor $S_m(k)$ along the x axis for a ground state prepared on the 2×4 ladder [see Fig. 2(c)], obtained at the end of the third step using either a fully variational or the corresponding HyVA_{2→3} protocol (green), again using the same implementation time. In both panels, we include the result for the exact ground state (in black).

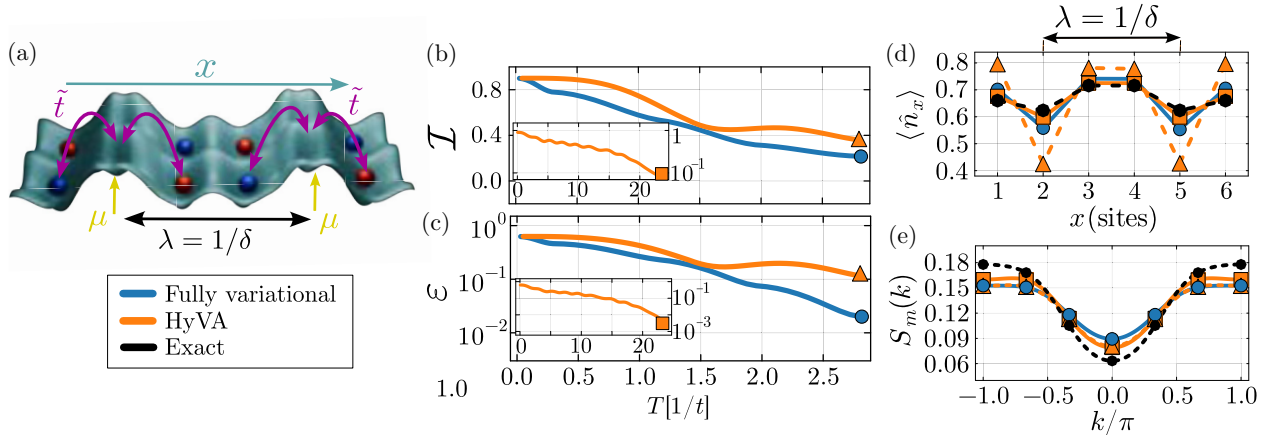


FIG. 4. Ground-state preparation for the local FH model at finite doping. (a) The initial state used to prepared the ground state of a 2×6 FH ladder with doping $\delta = 1/3$ and $U/t = 8$. Atoms are loaded into the optical lattice, with certain sites left empty according to the expected stripe configuration in the ground state, which has a wavelength $\lambda = 1/\delta$. (b),(c) The infidelity $\mathcal{I}$ and the residual energy ε , respectively, as a function of the implementation time T . We compare the results obtained with the variational circuit (blue) in Eq. (12) with the HyVA protocol (orange) described in the text. The insets show the results obtained with the latter for a longer adiabatic evolution time. (d),(e) The charge density profile $\langle \hat{n}_x \rangle$ and spin-structure factor along the x axis $S_m(k)$, respectively, for the final states prepared with these different methods. The markers indicate that the observables are obtained for the different times indicated in (b) and (c).

Fig. 3(b), we show the spin-structure factor,

$$S_m(k) = \sum_{ij} e^{ik(i-j)} \left[\langle \hat{S}_i^z \hat{S}_j^z \rangle - \langle \hat{S}_i^z \rangle \langle \hat{S}_j^z \rangle \right], \quad (11)$$

calculated along the x axis. For this observable, both the fully variational and the HyVA_{2→3} protocols produce similar results, confirming our previous conclusions. Here, we note that the extremely good performance of our protocols is partially a consequence of the relatively simple structure of the target ground state. We now demonstrate how these results are maintained for the more complicated case of an FH model with finite doping.

B. Fermi-Hubbard ladders at finite doping

In the presence of a finite doping δ , several works [49,115,116] have found that the ground state of $\hat{H}_{\text{FH}}$ forms charge stripes with a wavelength $\lambda_e = 1/\delta$, leading to one doped hole per unit cell. We now show how to prepare these doped ground states, which present a smaller energy gap as compared to the half-filled case studied above. In this case, we start with an antiferromagnetic product state of 8 fermionic atoms on a 2×6 ladder [see Fig. 4(a)], corresponding to $\delta = 1/3$. This state can be obtained experimentally by removing four atoms in nonconsecutive rungs of the ladder, starting from the state $|\Psi_0\rangle$ considered above for the half-filled case [8,14,15,98,117,118].

From this initial state, we prepare the ground state at $U/t = 8$ following two steps. First, we prepare the ground state of the dimers at the edge of the system as well as

the central 2×2 plaquette, using the precompiled variational circuits described above for the half-filled case. We then connect the dimers and plaquettes by applying the following parametrized unitary,

$$\mathcal{U}_\delta(\boldsymbol{\theta}) = \prod_{\mu=1}^D e^{-iT_\mu \hat{H}_\delta(\boldsymbol{\theta}_\mu)}, \quad (12)$$

with

$$\hat{H}_\delta = -\tilde{t} \sum_{\langle i,j \rangle \in \text{links}, \sigma} \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} - t \sum_{\langle i,j \rangle \notin \text{links}, \sigma} \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} \quad (13)$$

$$+ U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} + \Delta/t \sum_{i,\sigma} \mu_i \hat{n}_{i,\sigma} \quad (14)$$

and variational parameters $\boldsymbol{\theta}_\mu = (T_\mu \tilde{t}_\mu, T_\mu \Delta_\mu)$. Note that $\tilde{t}$ is now the tunneling for the links connecting dimers and plaquettes with their contiguous empty sites, and that we fix $\mu_i/t = 4$ for the initially empty sites and zero for the half-filled ones. This Hamiltonian can be implemented for larger systems in a translationally invariant manner while keeping δ fixed.

In Figs. 4(b) and 4(c), we plot ε and the $\mathcal{I}$ for the optimized circuit with $D = 2$ layers and compare the results with the ones obtained with a HyVA protocol. For the latter, the adiabatic fusion is now performed in two steps, first by ramping up from $\tilde{t} = 0$ to $\tilde{t} = t$, while keeping Δ fixed for a time T_1 , and then decreasing the chemical potentials until they are uniform along the ladder, for a time T_2 . From these results, we conclude that, similarly to the half-filled

case, the fully variational state preparation shows better performance in terms of both the fidelity and the accuracy of the energy estimation compared to the HyVA method for the same implementation time. However, the advantage of the latter relies on the fact that all the variational circuits are optimized classically and can thus be applied directly to an extended system. In the insets of the figure, we show how the results obtained with the HyVA protocol can be further improved by increasing the implementation time, which is still within the typical experimental coherence times. In the next section, we show how these results are maintained for larger system sizes.

In Fig. 4(d), we plot the charge-density profile along the x axis, $\langle \hat{n}_x \rangle$, to show that our variationally prepared states [at the times indicated by the markers in Fig. 4(b) and 4(c)] qualitatively reproduce the expected periodicity of the stripe pattern of the exact ground state. In the case of the HyVA protocol, longer implementations times are required for this, which is consistent with the results described above. Finally, the spin-structure factors along the x axis also agree for the states prepared with the different methods, as shown in Fig. 4(e). We note that while the quantitative agreement is not as good as for the half-filled case, our variational protocols approximate the properties of the exact ground state qualitatively for short implementation times. The difference here compared to half filling stems from the smaller gap and therefore longer correlation length of the target ground state.

C. Extended Fermi-Hubbard ladders

We finish this section by showing how our variational protocols can also be used to prepare the ground states of extended Fermi-Hubbard (eFH) models, where the target and resource Hamiltonians do not match. We illustrate our approach for the eFH model in the presence of NNN-tunneling terms,

$$\hat{H}_{\text{eFH}} = \hat{H}_{\text{FH}} + \hat{H}_{t'}, \quad (15)$$

with

$$\hat{H}_{t'} = -t' \sum_{\langle\langle i,j \rangle\rangle, \sigma} \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma}. \quad (16)$$

This model has regained significant interest because several works have suggested that these longer-range tunnelings stabilize a d -wave superconducting order in the thermodynamic limit [50,116,119]. However, the question is still not completely settled, since obtaining the ground state for large system sizes using classical methods is computationally very challenging [48]. This and other questions could be further investigated in fermionic cold-atom quantum simulators, where the d -wave order parameter can be efficiently measured experimentally [108].

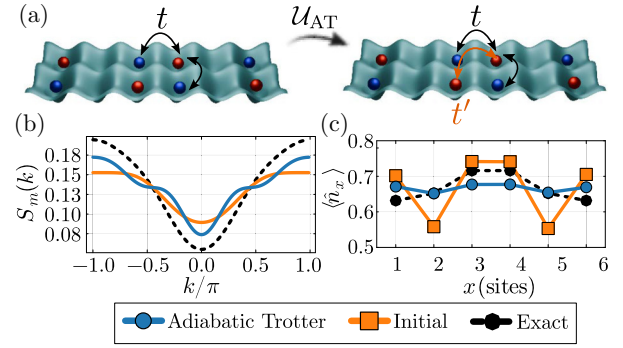


FIG. 5. The extended Fermi-Hubbard (eFH) model. (a) Using $\mathcal{U}_{\text{AT}}$, we prepare the ground state of the eFH model on a 2×6 ladder, for $U/t = 8$, $t/t' = -0.25$, and $\delta = 1/3$. As described in the text, we take as an initial state the ground state of the local FH model prepared with the HyVA protocol (orange), using a total time $Tt = 20$, and apply an adiabatic Trotter evolution for a time $T_{\text{Trotter}}t = 10$ to reach the target state (blue). (b),(c) The spin-structure factor $S_m(k)$ and the atomic density, respectively, calculated along the ladder. We show results for the initial and the prepared state and compare with the results obtained on the exact ground state of the model (in black).

We study, in particular, the eFH model given in Eq. (16) on a ladder geometry. We focus on the case with a finite doping of $\delta = 1/3$ and take $U/t = 8$ and $t'/t = -0.25$, a parameter regime that is compatible with the numerical evidence of d -wave superconducting order [116]. As initial state for the protocol, we consider the ground state of the local FH Hamiltonian, $|\psi_{\text{FH}}\rangle$, prepared with the protocols introduced in Sec. III B. We then transform this state to the ground state of the eFH model, $|\psi_{\text{eFH}}\rangle$, through an adiabatic Trotter (AT) evolution, where the NNN-tunneling terms are slowly introduced through a linear ramp, as schematically depicted in Fig. 5(a). In Appendix A, we show how to generate time evolutions under $\hat{H}_{t'}$ by just concatenating three unitaries from the fermionic gate set $\mathcal{G}$ given in Eq. (5), such that the whole protocol can be implemented using only local FH dynamics.

On a ladder geometry, this unitary evolution takes the form

$$\mathcal{U}_{\text{AT}} = \prod_k e^{-i\hat{H}_{\text{FH}} \frac{\Delta T}{2}} e^{-i\hat{H}_{t'}^{(1)} \frac{\Delta \tilde{T}_k}{2}} \times e^{-i\hat{H}_{t'}^{(2)} \Delta \tilde{T}_k} e^{-i\hat{H}_{t'}^{(1)} \frac{\Delta \tilde{T}_k}{2}} e^{-i\hat{H}_{\text{FH}} \frac{\Delta T}{2}}, \quad (17)$$

where $\Delta \tilde{T}_k = ((T_k + T_{k-1}) \Delta T) / (2T_{\text{Trotter}})$, $T_k = k \Delta T$, with k an integer and ΔT a suitable time step, and $0 < T_k \leq T_{\text{Trotter}}$. Here, $\hat{H}_{t'}^{(1)}$ and $\hat{H}_{t'}^{(2)}$ refer to the two sets of commuting operators in $\hat{H}_{t'}$, where we choose, in particular, the parallel diagonal terms along the two possible orientations in the ladder. Finally, we note that here the unitary time evolutions with NNN-tunneling terms, $e^{-i\hat{H}_{t'} \Delta T}$,

can be implemented using quench evolutions with only NN tunnelings, as described in Appendix A, such that the whole protocol can be implemented with the fermionic gate set given in Eq. (5). In this case, the application of the $\mathcal{U}_{\text{AT}}$ operator for a total time T_{Trotter} needs an equivalent physical time of $T = 2T_{\text{Trotter}}$.

In Fig. 5, we show the results obtained after applying this AT protocol to the initial state, $|\psi_{\text{FH}}\rangle$, obtained with the HyVA protocol described in Sec. III B for a total implementation time of $Tt = 20$. This state corresponds to the ground state of the local FH Hamiltonian prepared with a fidelity of approximately 87%. After its preparation, we implement $\mathcal{U}_{\text{AT}}$ for a total time of $T_{\text{Trotter}}t = 10$ and a time step $\Delta Tt = 0.05$, resulting in a final fidelity of approximately 86% for the exact ground state of the eFH model. In Figs. 5(b) and 5(c), we plot the spin-structure factor $S_m(k)$ given in Eq. (11) and the occupation numbers along the x axis, respectively, for the initial and the final states after the AT protocol. Our results show how, despite the imperfect state prepared due to Trotter errors arising from the Trotterization and also due to the finite value of T_{Trotter} used here, we can approximate the properties of the ground state of the extended model, which are qualitatively different from those in the initial state. Specifically, in this case, our protocol is able to melt the initial stripe order, as required to achieve a d -wave superconducting state.

The study of the emergence of such order is limited here by the system sizes that we can simulate classically. This and other properties of the phase diagram of the eFH model could be further investigated in a fermionic quantum simulator by applying the state-preparation protocols described here to larger system sizes. Finally, we note that the Trotter circuit can be shortened considerably by promoting the Trotter times to variational parameters, which could be optimized to reach similar fidelities in fewer Trotter steps. While performing this optimization classically is challenging for the system sizes considered here, this could be done directly in the quantum hardware through a VQE protocol.

IV. VARIATIONAL QUANTUM IMAGINARY-TIME EVOLUTION

In this section, we show how to approximate QITE on a fermionic quantum simulator using fermionic unitary circuits. Apart from being an alternative state-preparation method, QITE is an important subroutine for other quantum simulation algorithms, such as subspace expansion methods [120] or the algorithm recently introduced in Ref. [121] to estimate Loschmidt amplitudes. This last algorithm, through the possibility of performing QITE, could be used as a way to implement filtering algorithms [122–125] and statistical phase-estimation protocols [126–130] with fermionic quantum simulators.

Starting from some initial state $|\Phi(\tau = 0)\rangle$, the QITE protocol prepares the (nondegenerate) ground state of a target Hamiltonian $\hat{H}$,

$$|\Psi_{\text{GS}}\rangle = \lim_{\tau \rightarrow \infty} \frac{e^{-\tau \hat{H}} |\Phi(\tau = 0)\rangle}{\|e^{-\tau \hat{H}} |\Phi(\tau = 0)\rangle\|}, \quad (18)$$

provided that these two states have a nonzero overlap, i.e., $\langle \Psi_{\text{GS}} | \Phi(\tau = 0) \rangle \neq 0$. Implementing this protocol using quantum hardware is challenging, since it requires the application of a nonunitary operator. In Sec. IV A, we introduce a procedure to implement it in a fermionic quantum simulator by adapting a QITE algorithm that was first proposed for qubit-based devices [86], as well as its variational approximation (VarQITE) [87–89]. In Sec. IV B, we explain how to use the VarQITE protocol to construct an approximate Krylov subspace by postprocessing the collected data and then use it to obtain a better estimation of the energy using the QLanczos algorithm [86]. In Sec. IV C, we illustrate our protocols for the local FH model studied in Sec. III, as well as for an extended FH model with NN interactions. For the latter, the QITE protocol is implemented using only the local fermionic gate set given in Eq. (5), demonstrating that the proposed algorithms can be used to study target models different from the native experimental resources, by performing measurements on the quantum hardware and applying classical postprocessing. We finish this section by investigating the effect of shot noise on these algorithms and giving an estimation on the number of experimental repetitions required to run them with good precision on a cold-atom setup.

A. Approximating QITE with unitary evolutions

Given a target Hamiltonian $\hat{H}$, the goal of the protocol is to implement a variational approximation of the nonunitary QITE step,

$$|\psi(\tau + \Delta\tau)\rangle = c_\tau e^{-\Delta\tau \hat{H}} |\psi(\tau)\rangle, \quad (19)$$

where $\Delta\tau$ is the imaginary time step, $|\psi(\tau)\rangle$ is the imaginary-time-evolved state at time τ obtained after n QITE steps, with $|\psi(\tau = 0)\rangle$ some initial state, and $c_\tau = 1/\|e^{-\Delta\tau \hat{H}} |\psi(\tau)\rangle\|$ is a normalization constant. Although the QITE step is a nonunitary operation, since both $|\psi(\tau + \Delta\tau)\rangle$ and $|\psi(\tau)\rangle$ are normalized states, the two of them can be connected through the application of a unitary operator.

To find an approximation of this operator, and similar to other variational approaches, the idea is to define a parametrized quantum state $|\psi(\theta(\tau))\rangle$, prepared through a variational quantum circuit constructed using quenched unitary dynamics as described in Sec. III and characterized by a vector of tunable parameters $\theta(\tau) \in \mathbb{R}^d$. In Ref. [88], the imaginary time dynamics of the parameters

at a time τ are derived from McLachlan's variational principle. However, as explained in Appendix E, the required measurements are challenging to obtain with a fermionic optical-lattice simulator. For this reason, in Appendix E we develop an iterative approach similar to the one proposed in Ref. [86], where we instead approximate each time step using the following variational state:

$$|\psi(\boldsymbol{\theta}(\tau + \Delta\tau))\rangle = \prod_{\mu=1}^D e^{-iT_\mu \hat{H}_\mu} |\psi(\boldsymbol{\theta}(\tau))\rangle, \quad (20)$$

where $\hat{H}_\mu$ are the different terms of the Hamiltonian, e.g., $\hat{H}_\mu \in \{\hat{H}_t, \hat{H}_U\}$ for the local FH model. The state is thus updated by a sequence of global quenches with variational parameters $\theta_\mu(\tau) = T_\mu \lambda_\mu$, with $\lambda_\mu \in \{t, U\}$, corresponding to the fermionic gates in $\mathcal{G}$ given in Eq. (5). We refer to this approach as a variational QITE (VarQITE).

Setting the variational parameters to zero at each step, the quantities that need to be measured in the quantum hardware to update the variational parameters are the following:

$$\begin{aligned} g_{\mu\nu}(\boldsymbol{\theta}(\tau)) &= \text{Re} \left[\langle \hat{H}_\mu \hat{H}_\nu \rangle_{\boldsymbol{\theta}} \right] - \langle \hat{H}_\mu \rangle_{\boldsymbol{\theta}} \langle \hat{H}_\nu \rangle_{\boldsymbol{\theta}}, \\ b_\mu(\boldsymbol{\theta}(\tau)) &= \text{Im} \left[\langle \hat{H}_\mu \hat{H} \rangle_{\boldsymbol{\theta}} \right], \end{aligned} \quad (21)$$

where Re and Im denote the real and imaginary part, respectively. These observables can be measured in a cold-atom setup using state-of-the-art techniques, either globally including extra pulse sequences [108] or through parallelized measurements with the superlattice, as explained in Appendix C. We note that although the number of terms that we have to measure scale with the system size, making this protocol more challenging than the precompiled variational circuits described in the previous section, each of them can be obtained using current experimental techniques [57].

B. Using VarQITE to improve energy estimation through QLanczos

Let us now explain how the VarQITE can be used as a subroutine for more complex algorithms. One example is the QLanczos algorithm [86], a quantum version of the classical iterative Lanczos algorithm that can be used to significantly improve the energy estimated in the state prepared by the VarQITE.

The classical Lanczos algorithm [131] constructs a Hamiltonian $\mathbb{H}$ projecting $\hat{H}$ over a Krylov subspace $\{|\psi(0)\rangle, \hat{H}|\psi(0)\rangle, \hat{H}^2|\psi(0)\rangle, \dots\}$, where $|\psi(0)\rangle$ is an initial state. Diagonalizing $\mathbb{H}$ yields a variational estimate of the ground state that can be used to reinitialize the algorithm, improving the convergence with each iteration. The key idea of the quantum version of this algorithm, the

QLanczos, is to project the target Hamiltonian $\hat{H}$ into the Krylov subspace spanned by $|\psi(\tau_\alpha)\rangle$,

$$\mathbb{H}_{\alpha,\beta} = \langle \psi(\tau_\alpha) | \hat{H} | \psi(\tau_\beta) \rangle \quad (22)$$

at different imaginary times $\tau_\alpha = \alpha \Delta\tau$, with $\alpha = 1, \dots, N$. Using this projection, we can write the effective Schrödinger equation in the Krylov subspace, $\mathbb{H}|\Psi\rangle = E\mathbb{S}|\Psi\rangle$, where $\mathbb{S}$ is the matrix that takes into account the normalization,

$$\mathbb{S}_{\alpha,\beta} = \langle \psi(\tau_\alpha) | \psi(\tau_\beta) \rangle. \quad (23)$$

To understand intuitively why the states $|\psi(\tau_\alpha)\rangle$ obtained after α QITE steps are expected to generate a Krylov subspace, we can rewrite them from Eq. (19) as

$$|\psi(\tau_\alpha)\rangle = c_\alpha \left(e^{-\tau \hat{H}} \right)^\alpha |\psi(0)\rangle, \quad (24)$$

where $c_\alpha = \prod_{\tau=1}^\alpha c_\tau$ is the product of all the previous normalization factors. From that equation, we can conclude that the QITE steps create a Krylov-like subspace with iterative applications of the operator $e^{-\tau \hat{H}}$ instead of the bare $\hat{H}$.

The matrices $\mathbb{H}$ and $\mathbb{S}$ can be extracted using the quantum simulator in two different ways. First, as detailed in Appendix E, one can measure $|\mathbb{S}_{\alpha,\beta}|$ and $|\mathbb{H}_{\alpha,\beta}|$ directly by reversing the corresponding variational circuits and then follow the ideas described in Ref. [121] to obtain the corresponding phase. We refer to this approach as the *complete* QLanczos algorithm. Alternatively, one can obtain these matrices approximately using the recursive formula (for an explicit derivation, see Appendix E)

$$\begin{aligned} \mathbb{S}_{\frac{\alpha+1}{2}, \frac{\beta+1}{2}} &= c_\alpha c_\beta / c_{\frac{\alpha+\beta}{2}}^2, \\ \mathbb{H}_{\frac{\alpha+1}{2}, \frac{\beta+1}{2}} &= \mathbb{S}_{\frac{\alpha+1}{2}, \frac{\beta+1}{2}} \langle \psi(\tau_{\frac{\alpha+\beta}{2}}) | \hat{H} | \psi(\tau_{\frac{\alpha+\beta}{2}}) \rangle, \end{aligned} \quad (25)$$

where c_α are the normalization constants that can be obtained recursively at each step, by setting $c_1 = 1$ and

$$c_{\alpha+1}^2 = \frac{1 - 2\Delta\tau \langle \psi(\tau_\alpha) | \hat{H} | \psi(\tau_\alpha) \rangle}{c_\alpha^2} + \mathcal{O}(\Delta\tau^2). \quad (26)$$

The advantage of this approximation, which we denote as *approximated* QLanczos, is that it only relies on the measurement of $\langle \psi(\tau_\alpha) | \hat{H} | \psi(\tau_\alpha) \rangle$. Therefore, the steps to implement the approximated QLanczos involve the implementation of the QITE algorithm first and the consequent construction of the matrices $\mathbb{H}$ and $\mathbb{S}$ following Eqs. (25) and (26), where only data corresponding to the energy measurements obtained during the QITE algorithm are used. In contrast, implementing the full QLanczos approach requires an explicit calculation of $\mathbb{H}$ and $\mathbb{S}$

according to Eqs. (22) and (23), which, in general, involves the measurement of complex phases. This would need either the application of inverse circuits and the measurement of Loschmidt amplitudes [121] or the use of methods based on circuit perturbations [132].

Let us also mention that even though this approximation relies on a small time step $\Delta\tau$ to reach a good accuracy, the number of measurements required to calculate VarQITE scales with $1/\Delta\tau$, so this time step cannot be made arbitrary small. In Appendix E, we explain in detail how to measure the required quantities for these two methods in a cold-atom setup.

C. Application of VarQITE and QLanczos to Fermi-Hubbard ladders

We now apply the VarQITE and the different QLanczos protocols discussed above to the FH ladder with $U/t = 8$, both at half filling and for finite dopings. Moreover, we also consider the effect of NN-interaction terms. We investigate the performance of these methods as a function of the system sizes and for different choices of the initial state $|\psi(\tau = 0)\rangle$, which can be prepared with the variational protocols described in Sec. III. As shown in Ref. [86], the initial state should have a sufficiently good overlap with the target ground state, while at the same time have a moderate correlation length such that the nonunitary QITE step can be approximated by a unitary operator. For these reasons, we choose (i) a tensor product of the ground state of the FH model at $U/t = 8$ for each uncoupled plaquette and (ii) a similar plaquette product state but obtained for $U/t = 32$ to reduce the initial correlation length.

1. Local Fermi-Hubbard ladders

Our results for the local FH ladder are summarized in Fig. 6, where we first show the expectation value of the target Hamiltonian $\langle\hat{H}\rangle$ over the states evolved with our VarQITE protocol for a 2×12 ladder at half filling and compare them with the equivalent exact ITE calculation [dark dashed lines in Fig. 6(a)]. These results show the importance of the choice of the initial state. In particular, if we take the plaquette product state for $U/t = 8$ as the initial state (in solid blue), the protocol does not provide a significant improvement in the energy because the QITE step has a support (i.e., the number of fermion modes in which it acts simultaneously) smaller than the correlation length of the system and thus it cannot properly capture the imaginary-time dynamics [86]. In the language of variational quantum computing, we would say that the circuit lacks expressibility for that given initial state. On the other hand, for the initial plaquette product state with $U/t = 32$, which has a smaller overlap with the exact ground state, the protocol results in a larger improvement of the initial energy during the optimization. These results exemplify a trade-off between the trainability of the circuit and the

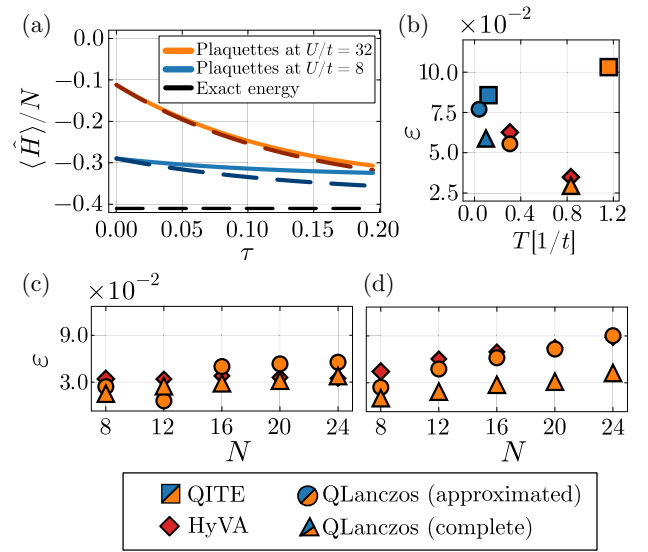


FIG. 6. VarQITE and QLanczos for the local FH ladder. (a) A comparison between the QITE protocol (solid lines) and the exact ITE (dashed lines) to prepare the ground state of a half-filled 2×12 ladder at $U/t = 8$, starting from different initial states depicted with different colors (see the text). The data were obtained updating the wave function according to Eq. (19) using $\Delta\tau = 0.005$. (b) We show the best residual energies ε obtained with the QITE protocol as well as with the two QLanczos methods, together with the required implementation time T , for the different initial states. We also show results obtained with the HyVA method (see Fig. 2) using the same implementation time. (c),(d) The results obtained for ε using the different protocols as a function of the ladder length N , for the case of half filling (c) and quarter filling (d), respectively.

quality of the initial state. Although a reduced expressibility improves the trainability of a variational quantum circuit [133], this needs to be accompanied by a suitable initial state. In such case, issues in the trainability can be solved while still being able to reach the states of interest in the Hilbert space [114,134].

Similarly to the HyVA protocol introduced in the previous section, our results show how our VarQITE approach can prepare the ground state of the FH Hamiltonian much faster than standard adiabatic protocols. As shown in Fig. 6(b), the bare application of VarQITE does not provide an advantage over the HyVA approach, considering, in particular, that it requires more complicated measurements. However, as we have mentioned previously, it can be used as a subroutine for other algorithms, such as QLanczos. We now show how this approach provides an advantage with respect to the HyVA protocol both in terms of implementation times as well as in the accuracy of the estimated ground-state energy.

In Figs. 6(b)–6(d), we summarize our results using the two QLanczos approaches described above. First, in Fig. 6(b), we plot the residual energy ε as a function of the total implementation time T and compare the results

obtained directly from the VarQITE algorithm [shown in Fig. 6(a)] and the ones obtained from the QLanczos algorithms [the circle (triangle) markers correspond to the approximated (complete) method]. We note that the physical time T that we are plotting in the horizontal axis in Fig. 6(b) is different for the different states considered, although the imaginary time [the horizontal axis in Fig. 6(a)] is the same in all cases. We also benchmark these protocols against the HyVA state preparation introduced in the previous section by showing, in each case, results obtained for the same total implementation times (in red rhombus). From these results, we can first conclude that both QLanczos protocols improve the energy with respect to the VarQITE algorithm from which the information is extracted and, more importantly, that they considerably reduce the evolution time required for that, since only short imaginary times are required. Moreover, for this system size, QLanczos performs better if the corresponding VarQITE starts with the plaquette state at $U/t = 32$ (orange lines and markers), even if the final energy obtained with the latter is worse than for the initial plaquette state at $U/t = 8$ (blue lines and markers). The reason is that the former has a shorter correlation length than the latter and better approximates the exact QITE for short times. This observation shows a trade-off between the fidelity of the initial state used for the QITE and the accurate approximation of the exact ITE. Whereas increasing the former may lead to a better final energy after the application of the QITE protocol while needing shorter times, as shown in Fig. 6(b), the latter guarantees that QLanczos will later provide a faster convergence to the exact energy. Finally, we also observe how, for this system size, both versions of the QLanczos algorithm introduced above perform better than the HyVA protocol for an equivalent implementation time.

In Fig. 6(c), we make a systematic analysis of the QLanczos advantage over the HyVA protocol for increasing ladder sizes, i.e., $N = 2 \times L$, where L is the length of the ladder. For the half-filled case, we can observe that the approximated QLanczos version shows worse performance compared to the HyVA protocol after a certain system size N . For the complete QLanczos, the performance is similar to that of the HyVA protocol. This behavior can be explained by the nature of the state that we are trying to prepare. At half filling, the gap of the system is very large and the adiabatic fusion of plaquettes is expected to be efficient even for short implementation times. The situation changes, however, if we now compare the performance of these protocols in the presence of doping. The results are shown Fig. 6(d), where we perform a similar scaling analysis of the performance of QLanczos against the HyVA protocol for the case of quarter filling. In that case, we now find a clear advantage of the complete QLanczos compared with the HyVA protocol that is maintained, and even increases, as the system size grows.

2. Fermi-Hubbard ladder with extended interactions

One of the main advantages of implementing the VarQITE and the QLanczos protocols is that there is no need to directly engineer all the terms in the target Hamiltonian $\hat{H}$ to estimate its ground-state energy. This is because the unitary parametrization [cf. Eq. (20)] of the nonunitary QITE step [cf. Eq. (19)] does not need to include, in principle, all the different terms in $\hat{H}$, the Hamiltonian generating the ITE. To illustrate this point, we now include an extra NN-interaction term to the half-filled FH ladder target Hamiltonian,

$$\hat{H}_V = V \sum_{(i,j)} \hat{n}_i \hat{n}_j, \quad (27)$$

where we set $V/t = 2$. We apply our protocols to this extended FH ladder and summarize our results in Fig. 7. In this case, both the initial states and the quench evolutions in the fermionic circuits are the same as above. The only difference is that now the observables that we have to measure in Eq. (21) also include the new term $\hat{H}_V$, as part of $\hat{H} = \hat{H}_{\text{FH}} + \hat{H}_V$.

In Fig. 7(b), we show the results obtained after implementing the VarQITE protocol starting from the same initial states as in Fig. 6(a). There, we demonstrate that we can accurately approximate the exact QITE corresponding to the extended FH Hamiltonian for the chosen parameter regimes. Furthermore, in Fig. 7(c), we perform a similar system-size analysis as in the local FH case. We find that

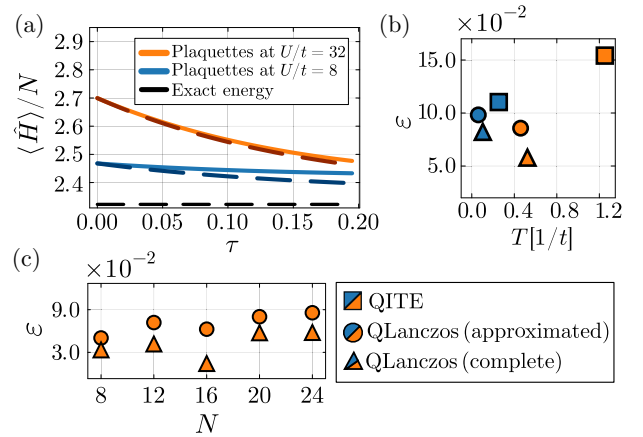


FIG. 7. VarQITE and QLanczos for the FH ladder with extended interactions. (a) A comparison between the QITE protocol (solid lines) and the exact ITE (dashed lines) to prepare the ground state of a half-filled 2×12 ladder at $U/t = 8$ and $V/t = 2$, starting from different initial states (see legend). (b) The best residual energies ϵ obtained with the QITE protocol as well as with the two QLanczos methods, together with the required implementation time T , for the different initial states. (c) The residual energies ϵ as a function of the ladder length N for the different protocols.

QLanczos still provides an advantage both in its approximate and its complete form when compared to the regular VarQITE and that these results hold as the system size increases. We note that, in this case, we do not assume that the term $\hat{H}_V$ is generated on the quantum simulator. Therefore, and since there is no equivalent adiabatic preparation, our results show how both the VarQITE and the QLanczos protocols developed here can be used to explore target models beyond the ones engineered in the experiment.

3. Effect of shot noise

Finally, let us note that all the results shown for the VarQITE and the QLanczos algorithms so far assume an infinite number of measurements. We now conclude this study by investigating how our protocols are affected by the presence of shot noise stemming from a finite number of samples in the estimation of each measured object. In Fig. 8(a), we compare the results obtained from the VarQITE algorithm for different number of samples, showing how the protocol is still able to capture the results obtained using an infinite number of measurements. Then, in Fig. 8(b), we show the final estimation of the energy provided by the approximated and complete versions of QLanczos as a function of the number of samples. The main conclusion is that a reasonable amount of total samples in the calculation of each object needed for QLanczos recovers the same values that were obtained in the infinite-measurement case. Therefore, based on the results discussed in the previous sections, we can conclude that QLanczos provides a good estimation of the energy of the ground state while requiring less coherence time than other methods, even in the presence of shot noise.

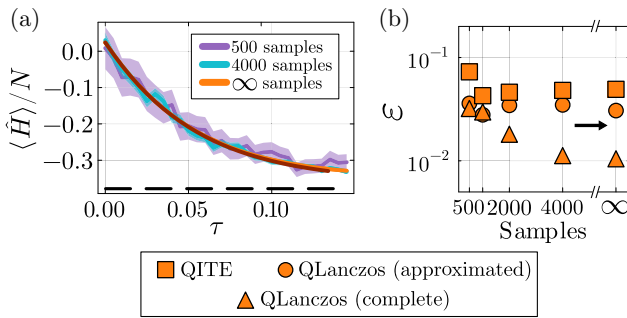


FIG. 8. The effects of shot noise in QITE and QLanczos. (a) A comparison between the QITE (solid lines) and the exact imaginary-time evolution (dashed lines) applied to the target local FH model with $U/t = 8$ in a 2×4 ladder, considering as initial state the uncoupled plaquettes with reduced t in Fig. 6(a). Each line considers a different number of samples per object, with the shaded ribbon being the standard deviation. (b) The best residual energies ϵ compared with the number of samples per object used to obtain them when considering the situation depicted in (a).

The number of required samples can be connected to the number of experimental runs needed to implement the algorithms in practice. Assuming that the required observables are measured following the parallelization schemes proposed in Appendix C, the number of experimental runs needed to implement a single VarQITE step grow as $\mathcal{O}(8NM)$ for a ladder, with N being the total number of sites and M the number of samples assumed in the calculation [$\mathcal{O}(10NM)$ for a full lattice]. Assuming the possibility to implement in parallel approximately ten independent 2D experiments, either within the same 2D layer [135] or using a three-dimensional optical lattice [136–138], the results shown above for a 2×4 ladder and $M = 2000$ samples per object can be obtained with approximately 1.5×10^4 experimental runs in total. This is within reach considering the repetition rates of current cold-atom experiments [110,139]. We note that this number can be further reduced by implementing more sophisticated measurement schemes based on quantum control techniques [108] or randomized protocols [140–145].

V. CONCLUSIONS AND OUTLOOK

In summary, we have shown how cold atoms in optical lattices can be operated as programmable quantum simulators of fermionic models, where we harness the latest experimental advances demonstrating local control of these platforms. Here, we focus on ground-state preparation and develop quantum algorithms that overcome some of the limitations of more traditional analog quantum simulation approaches.

We first construct hybrid variational-adiabatic protocols that are precompiled classically and demonstrate that they can faithfully prepare the ground state of translational-invariant local and extended FH models, both at half filling as well as for finite dopings. Importantly, we show that these precompiled circuits require considerably less time than adiabatic protocols. Besides, we also demonstrate that they can be used to study models beyond the local FH models used as resources, e.g., FH with extended tunneling terms, required to obtain a d -wave superconducting order. Second, we propose how to obtain a variational approximation of the quantum imaginary-time evolution using resources available in cold-atom setups and benchmark its potential as an alternative state-preparation strategy for fermionic Hamiltonians. Finally, we also show that this protocol can be used as a subroutine for the QLanczos algorithm, which only requires postprocessing of the data measured during imaginary-time evolution, and demonstrate how it considerably improves the ground-state energy estimation for local and extended FH models. While we benchmark our protocols on ladder geometries, they are designed for extended 2D systems and can readily be applied to cold-atom experiments to investigate system sizes that cannot be addressed using classical methods.

The fermionic gate set considered in this work can be extended by including more general resources that can be natively implemented in cold-atom simulators, such as synthetic gauge fields [146] or long-range interactions [147–149]. The former would allow to target fractional quantum Hall states [150], which are topologically ordered phases that are very hard to prepare adiabatically due to gap-closing transitions, and the latter could help to prepare critical states more efficiently [151].

Besides these specific applications to ground-state preparation, our programmable quantum simulation approach can be used to design and implement other quantum algorithms tailored to cold-atom experiments. The fermionic gate set given in Eq. (5) introduced here can be readily used to implement a Trotter real-time evolution under extended FH dynamics. Furthermore, these resources can be also employed to construct more efficient many-body spectroscopy methods to better estimate the properties of the fermionic states prepared here, a research direction that we will explore in future works.

ACKNOWLEDGMENTS

D.G.-C. acknowledges support from the European Union (EU) Horizon Europe program under the Marie Skłodowska Curie Action PROGRAM (Grant No. 101150724). C.T. acknowledges support from Comunidad de Madrid (PIPF-2022/TEC-25625) and also from the Fundación Humanismo y Ciencia. C.T. and A.G.T. acknowledge support from the the Spanish National Research Council (CSIC) Research Platform on Quantum Technologies PTI-001, and from Spanish project PID2021-127968NB-I00 funded by the Ministry of Science, Innovation and Universities (MICIU)-State Research Agency (AEI) 10.13039/501100011033, and from the QUANTERA project MOLAR with reference PCI2024-153449 and funded by MICIU–AEI 10.13039/501100011033 and by the EU. This research was supported in part by National Science Foundation (NSF) Grant No. PHY-2309135 to the Kavli Institute for Theoretical Physics (KITP). The numerical calculations in this paper were performed using the ITensor package [152] and were run on the FinisTerae supercomputer supported by the Centro de Supercomputación de Galicia (CESGA). Work in Innsbruck was supported by the EU Horizon Europe programs HORIZON-CL4-2022-QUANTUM-02-SGA via the project 101113690 (PASQuanS2.1). C.K. acknowledges support from the NSF through a grant for the ITAMP at Harvard University.

DATA AVAILABILITY

The data that support the findings of this paper are openly available [153,154].

APPENDIX A: PROGRAMMING EXTENDED FERMION-HUBBARD MODELS

In this appendix, we show how, by implementing a sequence of quench evolutions corresponding to the fermionic gate set $\mathcal{G}$ given in Eq. (5), it is possible to generate evolutions under more complicated Hamiltonians beyond the local FH model given in Eq. (1). While here we focus on the implementation of the NNN-tunneling term of Eq. (16), other extended terms can be also obtained in a similar manner.

One key element to achieve this task is the implementation of fermionic SWAP (fSWAP) gates between two NN sites i and j , i.e., $\text{fSWAP}_{i \leftrightarrow j} |a\rangle_i |b\rangle_j = |b\rangle_i |a\rangle_j$, where $|a\rangle$ and $|b\rangle$ are the different atomic states, with $a, b \in \{0, \uparrow, \downarrow, \uparrow\downarrow\}$. These gates can be directly implemented by dimerizing the lattice, as described in Fig. 1(a), and applying an off-site chemical potential such that the system evolves under the Hamiltonian

$$\hat{H}_{\text{fs}} = -t \sum_{\sigma} \left(\hat{c}_{i,\sigma}^{\dagger} \hat{c}_{j,\sigma} + \text{H.c.} \right) - 3t (\hat{n}_{i,\sigma} + \hat{n}_{j,\sigma}), \quad (\text{A1})$$

for a total time $T_{\text{fs}} = \pi/(2t)$ [25] [see Fig. 9(a)]. Using the superlattice structures shown in Fig. 1(a), this gate can be parallelized for all dimers in the lattice, and alternated in different directions to generate more complex evolutions.

In Fig. 9(b), we schematically depict how to obtain unitary evolutions under the NNN-tunneling Hamiltonian in a plaquette through a sequence of fSWAP gates and dimerized tunnelings. Specifically,

$$e^{-i\hat{H}_{t'}T'} = \text{fSWAP}_{j \leftrightarrow k} e^{-i\hat{H}^{(1)}T} \text{fSWAP}_{j \leftrightarrow k}, \quad (\text{A2})$$

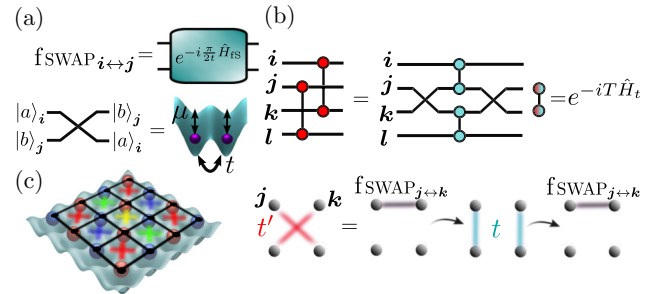


FIG. 9. Fermionic circuits for extended tunneling, (a) a fermionic SWAP (fSWAP) gate can be implemented between two NN sites i and j by evolving with the Hamiltonian $\hat{H}_{\text{fs}}$ given in Eq. (A1) for a time $\pi/(2t)$. (b) A unitary evolution under NNN-tunneling terms $\hat{H}_{t'}$ (red, diagonal in the plaquette) can be implemented using a sequence of fSWAP gates and quench evolutions under the NN-tunneling Hamiltonian $\hat{H}_t$ (blue) for a time $tT = t'T'$. (c) A sequential application of the operations described in (b) to the four sets of noncommuting plaquettes generates an effective evolution under NNN-tunneling terms along the whole lattice.

where $e^{-i\hat{H}^{(1)}T}$ corresponds to a quench evolution for a lattice configuration with vertical tunnelings [see Fig. 1(a)] and $tT = t'T'$. This protocol can be applied in parallel to all commuting plaquettes in the lattice [see Fig. 9(c)] and, thus, by repeating it four times, we can implement the unitary evolution under the NNN-tunneling Hamiltonian on the whole lattice. We note that this circuit has a finite depth, independent on the system size.

APPENDIX B: RESOURCE HAMILTONIANS FOR PRECOMPILED VARIATIONAL CIRCUITS

Here, we write down explicitly the resource Hamiltonians used in Sec. III to prepare the ground state of the FH model at half filling. For the first step of the protocol, the variational circuit given in Eq. (8) is obtained by quenching with the following Hamiltonian:

$$\hat{H}^{(1)} = -t \sum_{(i,j) \in \text{dimers}, \sigma} \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} - \mu \sum_i (-1)^{i_x + i_y} (\hat{n}_{i,\uparrow} - \hat{n}_{i,\downarrow}), \quad (\text{B1})$$

where the tunneling is nonzero only between pairs of sites within dimers, as depicted in Fig. 2(b), and we optimize t , U and μ for each quench.

In the second step, we start with the dimer product state prepared variationally and construct a second variational circuit by quenching with the Hamiltonian [see Fig. 2(c)]

$$\hat{H}^{(2)} = -\tilde{t} \sum_{(i,j) \in \text{rungs}, \sigma} \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} - t \sum_{(i,j) \in \text{dimers}, \sigma} \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow}, \quad (\text{B2})$$

where in this case we fix $U/t = 8$ and consider only $\tilde{t}_\mu$ and the quench time $T_\mu^{(2)}$ as variational parameters. Finally, in the third step, we apply the Hamiltonian $H^{(3)}$, which is similar to Eq. (B2), but with $\tilde{t}$ and t now referring to the interplaquette and intraplaquette couplings, respectively.

APPENDIX C: MEASUREMENT SCHEMES

In this appendix, we show in detail how to measure $\langle \hat{H} \rangle$ for the local FH Hamiltonian, where $\langle \hat{H} \rangle = \langle \hat{H}_t \rangle + \langle \hat{H}_U \rangle$. Extended tunneling terms can be included in a similar manner, by bringing them first to an NN form using a constant-depth circuit of fSWAP gates, as explained in Appendix A. We also consider measurements of $\langle \hat{H}_\mu \hat{H}_v \rangle$, which are required to implement QITE. Both $\langle \hat{H}_U \rangle$ and $\langle \hat{H}_t^2 \rangle$ are diagonal in the occupation basis and can be measured in a straightforward manner using a quantum gas microscope [105–107]. We now consider the remaining terms separately. Finally, let us also note that these

measurements can also be performed using the protocol introduced in Ref. [108] and based on quantum optimal control.

1. Measurement of $\langle \hat{H}_t \rangle$

The first operator that we are interested in measuring is $\hat{H}_t$. When computed over a 2D square lattice, this operator can be divided into four commuting parts such that all the terms in each one of them can be measured simultaneously through the appropriate dimerization of the lattice. Labeling these commuting parts with the index α yields the decomposition

$$\hat{H}_t = -t \sum_\alpha \hat{H}_{t,\alpha} = -t \sum_\alpha \sum_{(i_\alpha, j_\alpha), \sigma} \hat{c}_{i_\alpha, \sigma}^\dagger \hat{c}_{j_\alpha, \sigma}, \quad (\text{C1})$$

where all the terms in each $\hat{H}_{t,\alpha}$ for different i_α and j_α commute. The measurement of each term $\hat{H}_{t,\alpha}$ can be performed by first applying the unitary operation

$$\mathcal{B}_\alpha = \bigotimes_{(i_\alpha, j_\alpha), \sigma} \mathcal{B}_{i_\alpha, j_\alpha, \sigma}. \quad (\text{C2})$$

where each term $\mathcal{B}_{i_\alpha, j_\alpha, \sigma}$ brings the corresponding tunneling term to a diagonal form in the occupation basis, and they can all be applied in parallel for a fixed α , i.e.,

$$\begin{aligned} \langle \hat{H}_{t,\alpha} \rangle &= -\frac{t}{2} \sum_{(i_\alpha, j_\alpha), \sigma} \langle \hat{c}_{i_\alpha, \sigma}^\dagger \hat{c}_{j_\alpha, \sigma} + \hat{c}_{j_\alpha, \sigma}^\dagger \hat{c}_{i_\alpha, \sigma} \rangle_\psi \\ &= -\frac{t}{2} \sum_{(i_\alpha, j_\alpha), \sigma} \langle \hat{n}_{i_\alpha, \sigma} \rangle_\varphi - \langle \hat{n}_{j_\alpha, \sigma} \rangle_\varphi, \end{aligned} \quad (\text{C3})$$

where $|\varphi\rangle = \mathcal{B}_\alpha |\psi\rangle$. For a fixed α , all the terms $\langle \hat{H}_{t,\alpha} \rangle$ can thus be measured simultaneously using a quantum gas microscope, as shown experimentally in Ref. [57]. We note that in Eq. (C3), we have symmetrized each of the NN terms and thus the addition of the factor of 1/2.

Let us finally show that the $\mathcal{B}$ operator can be alternatively implemented in a compact manner by using two quench evolutions under the Hamiltonian

$$\begin{aligned} \hat{H}_{\text{FT}}(\theta_k) &= - \sum_\sigma \theta_{ij} \left(\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + \hat{c}_{j,\sigma}^\dagger \hat{c}_{i,\sigma} \right) \\ &\quad - \mu_{ij,1} \hat{n}_{i,\sigma} - \mu_{ij,2} \hat{n}_{j,\sigma}, \end{aligned} \quad (\text{C4})$$

where θ_{ij} , $\mu_{ij,1}$, and $\mu_{ij,2}$ are different variational parameters for each quench. We can optimize these parameters to minimize the infidelity $\mathcal{I}(\theta) = \|\mathcal{B} - e^{-i\hat{H}_{\text{FT}}(\theta_1)} e^{-i\hat{H}_{\text{FT}}(\theta_2)}\|$, where $\|\cdot\|$ is the Frobenius matrix norm. This protocol results in $\mathcal{I} < 10^{-8}$ for a wide range of parameters, which can potentially lead to a faster implementation compared to the $Z_{\pi/2}$ and $X_{\pi/2}$ rotations implemented in Ref. [57].

2. Measurement of $\langle \hat{H}_t^2 \rangle$

We now turn our attention to the measurement of $\langle \hat{H}_t^2 \rangle$, corresponding to a linear combination of $O(N^2)$ four-point correlation functions

$$\begin{aligned} \langle \hat{H}_t^2 \rangle &= \sum_{\langle i,j \rangle, \sigma} \sum_{\langle r,s \rangle, \sigma'} \langle \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} \hat{c}_{r,\sigma'}^\dagger \hat{c}_{s,\sigma'} \rangle \\ &= \frac{1}{4} \sum_{\langle i,j \rangle, \sigma} \sum_{\langle r,s \rangle, \sigma'} \left\langle \left(\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + \text{H.c.} \right) \left(\hat{c}_{r,\sigma'}^\dagger \hat{c}_{s,\sigma'} + \text{H.c.} \right) \right\rangle. \end{aligned} \quad (\text{C5})$$

We now introduce a measurement scheme for these terms and how it can be parallelized.

Let us first consider the case in which the following conditions are satisfied: (1) i and j are both different of r and s ; (2) $\sigma \neq \sigma'$; or (3) $i = r, j = s$ and $\sigma = \sigma'$. In that case, it is possible to independently apply an operator $\mathcal{B}_{i,j} \otimes \mathcal{B}_{r,s}$ that simultaneously diagonalizes each term in parentheses in Eq. (C5). Let $|\varphi\rangle = \mathcal{B}_{i,j} \otimes \mathcal{B}_{r,s} |\psi\rangle$. Then,

$$\begin{aligned} &\left\langle \left(\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + \text{H.c.} \right) \left(\hat{c}_{r,\sigma'}^\dagger \hat{c}_{s,\sigma'} + \text{H.c.} \right) \right\rangle_\psi \\ &= \langle (\hat{n}_{i,\sigma} - \hat{n}_{j,\sigma}) (\hat{n}_{r,\sigma'} - \hat{n}_{s,\sigma'}) \rangle_\varphi \end{aligned} \quad (\text{C6})$$

and the correlation functions can be computed with measurements over the occupation basis. Furthermore, $O(N)$ of these measurements can be parallelized, so the total number of configurations that need to be measured is of order $O(N)$.

There are still $O(N)$ observables that remain to be measured, namely, when i or j equal r or s (not both) and $\sigma = \sigma'$. Let $j = r$, without loss of generality. In that case, each of the terms to measure in Eq. (C5) can be rearranged as

$$\begin{aligned} &\left(\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + \hat{c}_{j,\sigma}^\dagger \hat{c}_{s,\sigma} + \text{H.c.} \right)^2 \\ &= \left(\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + \text{H.c.} \right)^2 + \left(\hat{c}_{j,\sigma}^\dagger \hat{c}_{s,\sigma} + \text{H.c.} \right)^2 \\ &\quad + \left(\hat{c}_{j,\sigma}^\dagger \hat{c}_{s,\sigma} + \text{H.c.} \right) \left(\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + \text{H.c.} \right) \\ &\quad + \left(\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + \text{H.c.} \right) \left(\hat{c}_{j,\sigma}^\dagger \hat{c}_{s,\sigma} + \text{H.c.} \right). \end{aligned} \quad (\text{C7})$$

The term $\mathcal{D}_{ij\sigma\sigma} = \left(\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + \text{H.c.} \right)^2 + \left(\hat{c}_{j,\sigma}^\dagger \hat{c}_{s,\sigma} + \text{H.c.} \right)^2$ is already measured in the different permutations considered above, so the only task left is the measurement of the second line in Eq. (C7). To do so, one may note that $\hat{c}_{j,\sigma}^\dagger \hat{c}_{s,\sigma} \hat{c}_{j,\sigma}^\dagger \hat{c}_{i,\sigma}$, $\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma}$ and their Hermitian conjugates are all equal to zero due to the fermionic

anticommutation rules. Hence, Eq. (C7) reads

$$\begin{aligned} &\left(\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + \hat{c}_{j,\sigma}^\dagger \hat{c}_{s,\sigma} + \text{H.c.} \right)^2 = \mathcal{D}_{ij\sigma\sigma} \\ &\quad + \left(\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} \hat{c}_{j,\sigma}^\dagger \hat{c}_{s,\sigma} + \hat{c}_{j,\sigma}^\dagger \hat{c}_{i,\sigma} \hat{c}_{s,\sigma}^\dagger \hat{c}_{j,\sigma} + \text{H.c.} \right) \\ &= \mathcal{D}_{ij\sigma\sigma} + \left(\hat{c}_{i,\sigma}^\dagger \hat{c}_{s,\sigma} + \text{H.c.} \right) (1 - 2\hat{n}_{j,\sigma}), \end{aligned} \quad (\text{C8})$$

where the final equality has been obtained after an application of the fermionic anticommutation rules. Thus, the procedure to measure Eq. (C8) consists in the simultaneous measurement of $\left(\hat{c}_{i,\sigma}^\dagger \hat{c}_{s,\sigma} + \text{H.c.} \right)$ and $\hat{n}_{j,\sigma}$, which can be achieved applying a $\text{fSWAP}_{s \leftrightarrow j}$ and then applying the corresponding $\mathcal{B}$ operator. Once again, most of these measurements can be parallelized, so it is possible to measure these terms in constant depth.

3. Measurement of $\text{Re} [\langle \hat{H}_t \hat{H}_U \rangle]$ and $\text{Im} [\langle \hat{H}_t \hat{H}_U \rangle]$

Finally, let us outline the measurement of the crossed terms, which are necessary for the QITE protocol in Sec. IV. For the first case, let us write $\text{Re} [\langle \hat{H}_t \hat{H}_U \rangle]$ as

$$\text{Re} [\langle \hat{H}_t \hat{H}_U \rangle] = \frac{1}{2} \langle \hat{H}_t \hat{H}_U + \hat{H}_U \hat{H}_t \rangle. \quad (\text{C9})$$

Since $\hat{H}_t$ and $\hat{H}_U$ are both Hermitian operators, the second equality in Eq. (C9) is the expectation value of an Hermitian operator. Decomposing these operators into observables that can be measured, we find that

$$\begin{aligned} &\langle \hat{H}_t \hat{H}_U + \hat{H}_U \hat{H}_t \rangle \\ &= \frac{1}{2} \sum_{\langle i,j \rangle, \sigma} \sum_s \left\langle \left(\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + \hat{c}_{j,\sigma}^\dagger \hat{c}_{i,\sigma} \right) \hat{n}_{s,\uparrow} \hat{n}_{s,\downarrow} + \text{H.c.} \right\rangle. \end{aligned} \quad (\text{C10})$$

There are two different types of terms arising from the above sum. First, there are the ones obtained when $i, j \neq s$. In such a case, it is possible to diagonalize the $\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + \hat{c}_{j,\sigma}^\dagger \hat{c}_{i,\sigma}$ term using a $\mathcal{B}_{i,j,\sigma}$ operator and then compute the expectation value as described in the above cases, measuring the products of number operators in the occupation basis. The measurement of these terms can be parallelized, so only $O(N)$ different configurations are needed to measure the $O(N^2)$ terms.

Second, there are also the terms where i or j equal s . Without loss of generality, let $j = s$. Then, these terms in

Eq. (C10) become

$$\begin{aligned} & \left\langle \left(\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + \hat{c}_{j,\sigma}^\dagger \hat{c}_{i,\sigma} \right) \hat{n}_{j,\uparrow} \hat{n}_{j,\downarrow} + \text{H.c.} \right\rangle \\ &= \left\langle \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} \hat{n}_{j,\uparrow} \hat{n}_{j,\downarrow} + \text{H.c.} \right\rangle \\ &= \left\langle \left(\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + \text{H.c.} \right) \hat{n}_{j,\sigma' \neq \sigma} \right\rangle. \end{aligned} \quad (\text{C11})$$

As in the previous cases, the tunneling term can now be diagonalized and hence measured.

Finally, regarding the measurement of $\text{Im} \left[\langle \hat{H}_t \hat{H}_U \rangle \right]$, we first rewrite this term as

$$\text{Im} \left[\langle \hat{H}_t \hat{H}_U \rangle \right] = -\frac{i}{2} \left(\langle \hat{H}_t \hat{H}_U - \hat{H}_U \hat{H}_t \rangle \right). \quad (\text{C12})$$

The operator to measure in the second equality of Eq. (C12) is Hermitian, and hence an observable. Its measurement is completely equivalent to the measurement of $\text{Re} \left[\langle \hat{H}_t \hat{H}_U \rangle \right]$ that was described above, with the only difference being that the measurement of each of the tunneling terms $\left(\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + \hat{c}_{j,\sigma}^\dagger \hat{c}_{i,\sigma} \right)$ is now a measurement of the current operator $i \left(\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} - \hat{c}_{j,\sigma}^\dagger \hat{c}_{i,\sigma} \right)$. Fortunately, such an operator can also be diagonalized with a $\mathcal{C}$ operator similar to the $\mathcal{B}$ that has diagonalized the tunneling term. As described in Ref. [57], this term can be easily obtained with a simple $X_{\pi/2}$ rotation.

APPENDIX D: EFFECTS OF NOISE IN THE IMPLEMENTATION OF THE VARIATIONAL PROTOCOLS

In this appendix, we discuss the effects of imperfect operations in the implementation of the variational protocols discussed in the main text. We take as a particular example Sec. III A and reproduce Fig. 2 including realistic errors.

Intuitively, the variationally optimized parameters minimize the value of a cost function, so the gradient there is zero and a small perturbation should not take the value of the cost function far away. Furthermore, since the number of parameters is kept of order $\mathcal{O}(1)$ but the number of degrees of freedom of the state scales exponentially and the circuit used is “physically inspired” (in the sense that, in the limit of $D \gg 1$ layers, one recovers a Trotterized adiabatic protocol), the cost function should not present lots of local minima, especially as the size of the system increases. Therefore, we expect the cost-function landscape (i.e., the value of $\langle \psi(\theta) | \hat{H} | \psi(\theta) \rangle$) to be smooth. Overall, this means that the cost function is not particularly sensitive to small changes in the values of the parameters around the minima.

Let us now provide a quantitative analysis to confirm this intuition of the robustness to noise of the protocol. In

Fig. 10, we reproduce Fig. 2 but including randomly sampled noise in each parameter. This models a situation in which the quenches cannot be perfectly implemented but instead have an intrinsic error associated. To do so, let the variational state obtained after quenching the state with the exact parameters obtained in the optimization (labeled as “Variational preparation” in Fig. 10) be $|\psi(\theta^*)\rangle$. Instead of preparing this state, we prepare $|\psi(\tilde{\theta}^*)\rangle$ adding Gaussian noise to the parameters as

$$\theta^* \rightarrow \tilde{\theta}^* = \theta^* + \epsilon, \quad \epsilon_i \sim \mathcal{N}(0, \sigma^2), \quad (\text{D1})$$

i.e., we randomly perturb each parameter sampling from a normal distribution with standard deviation σ^2 [these different levels of noise are labeled in Fig. 10 as Noise level = $(100 \times \sigma^2)\%$ to provide a percentage instead].

Furthermore, in order to increase the robustness of the overall protocol and ease a possible experimental implementation, the preparation of the dimers starting from the initial product state is done with quenches under the same Hamiltonian $\hat{H}^{(1)}$ that is used in Fig. 2 [cf. Eq. (B1)] but now with the value of U fixed to be $U/t = 8$ (the final objective value). Figures 10(a) and 10(b) show, respectively, the infidelity $\mathcal{I}$ and the residual energy ϵ obtained for this state preparation, including different values of the noise as described above for 50 independent random realizations (the results plotted are the corresponding means). The main conclusion is that although the perfect fidelities obtained in the noiseless protocol are now unreachable, a reasonable fidelity in the implementation of the operations (between 98% and 99%) already prepares the dimers with infidelities below 10^{-3} in much shorter times than their adiabatic counterparts.

For completeness, in Figs. 10(c) and 10(d) we show the results of preparing the plaquettes and in Figs. 10(e) and 10(f) the results for the 2×4 ladder. From these figures, we see that they are much more resilient to noise than the dimer preparation of Figs. 10(a) and 10(b). In particular, fidelities of 98% lead to infidelities of the prepared states below 10^{-3} , much closer to the noiseless values than in the dimer case. This is even more striking in the fusion of the plaquettes, where the noise hardly modifies the values of the figures of merit, even when only a 90% fidelity in the operations is considered. This situation, where the resilience to noise is improved as the system size increases, seems to provide numerical evidence to the intuition that a circuit with $\mathcal{O}(1)$ parameters will be more resilient to noise the bigger the underlying Hilbert space is.

Furthermore, in order to visualize better the effect of the random noise during the state preparation, in Fig. 11 we plot the same data as in Fig. 10 but now using a linear scale. This lets us introduce the standard deviation of the infidelity and the residual energy after the 50 independent realizations as a shaded ribbon in the panels. Moreover, the different scale clearly shows the oscillations in the energy

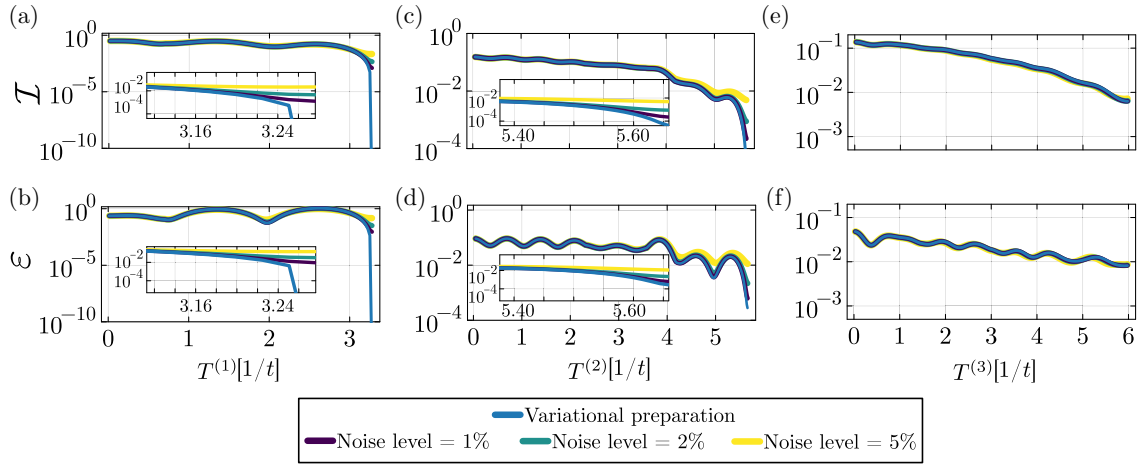


FIG. 10. The robustness against random noise in the parameters of the ground-state preparation for the local FH at half filling (logarithmic scale). This figure depicts a ground-state preparation equivalent to the one shown in Fig. 2 but including random noise in the parameters. The noise is included by sampling randomly from a normal distribution with mean the exact value and a standard deviation σ , such that the noise level in the labels is given as noise level = $100 \times \sigma^2\%$. The total number of random samples is 50. (a),(b) The infidelity and the residual energy, respectively, in the preparation of the dimer for the exact variational parameters and different values of noise. The inset shows the final times with an expanded scale. The optimization is different from the one considered in the main text, since it fixes the value of $U/t = 8$ instead of optimizing it to ease the experimental implementation of the protocol. (c),(d) We also show the infidelity and the residual energy, respectively, for the preparation of the plaquettes. In this case, the optimization has again been done with $D^{(2)} = 4$ layers, so the parameters obtained are different than the ones used in the main text. (e),(f) The same figures of merit, respectively, as the latter, in the case of the coupling of two plaquettes to prepare a 2×4 ladder.

and the infidelity and their robustness to noise. This phenomenon seems to indicate that the variational protocols provide better accuracy in the final-state preparation while needing much less time than their adiabatic counterparts, as discussed in Fig. 2. This improved performance can be associated with a transfer of population from the ground state to excited states, which may then be diabatically connected to the ground state through closing gaps (in, e.g., a similar way as the shortcut-to-adiabaticity protocol in Ref. [77] does).

Furthermore, to demonstrate that the variational protocol works with more realistic pulses and still provides a clear advantage, we have done calculations using linear ramps to switch the parameters on and off. The results are summarized in Fig. 12. The variational parameters in this new case are the ramping-time length and the value of the square pulse and its length. Thus, to couple the disconnected sites and prepare the dimers, we again quench the initial product state with the Hamiltonian $\hat{H}^{(1)}$ [cf. Eq. (B1)], fixing U to the target value ($U/t = 8$) and only

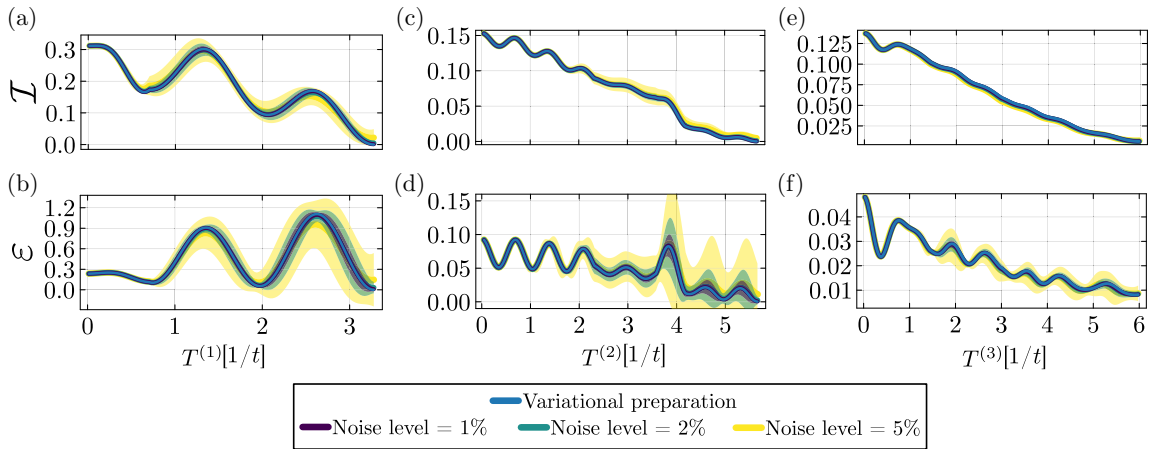


FIG. 11. The robustness against random noise in the parameters of the ground-state preparation for the local FH at half filling (linear scale). This figure is equivalent to Fig. 10 but in a linear scale instead of a logarithmic one. This allows the introduction of the standard deviation of all 50 averaged realizations for the noisy cases as a ribbon.

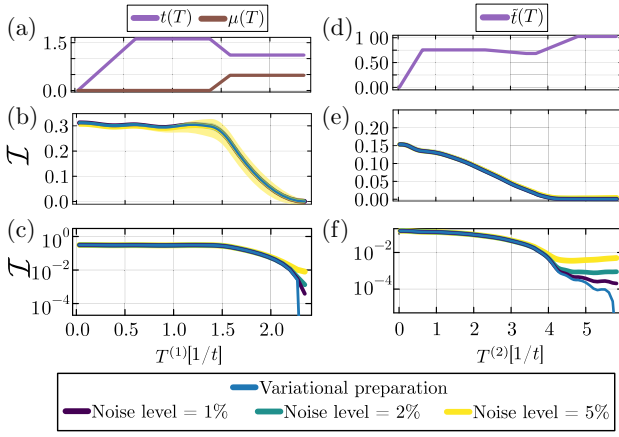


FIG. 12. The robustness of the variational state preparation with ramping pulses when noise is introduced. (a) The pulses used to prepare a dimer starting from a Mott-insulator state using two quenches of the Hamiltonian in Eq. (B1). The first quench ramps the tunneling t , which is then kept constant for some time. The second quench then ramps both t and μ , which are then kept constant again. (b) The infidelity $\mathcal{I}$ between the prepared state and the ground state of the FH model in a dimer as a function of the total time of the quenches. The figure shows the noiseless case (depicted as the variational one) and the average of 200 realizations with different levels of noise according to the colors (the ribbon corresponds to their standard deviation). (c) The same data as in (b) but plotted in a logarithmic scale. (d)–(f) The same as (a)–(c) but for the coupling of dimers to prepare the ground state of the plaquette, following three quenches of the system under the Hamiltonian in Eq. (B2), with their corresponding adiabatic ramps.

optimizing the values of t and μ together with the total quench duration and the ramping length. In Fig. 12(a), we show the optimal value of the pulses: we start by ramping the tunneling term t above the target value while keeping the value of μ at zero. In Fig. 12(b), almost no infidelity change is shown with respect to the dimers up to this point, so this can be considered as a nonadiabatic mechanism to move population between the excited states. Then, the value of t is adiabatically decreased and meanwhile the value of μ starts to increase. This is the moment at which the infidelity starts to decrease in Fig. 12(b) and it keeps decreasing while both of them are kept constant up until they reach a perfect state preparation in the ideal case. Moreover, we include different values of random Gaussian noise in the parameters following the same method as considered in Figs. 10 and 11 [cf. Eq. (D1)].

In Fig. 12(b), we plot the average value of 200 random realizations, together with their standard deviation as a ribbon. What we can see from this figure is that the values of the noise do not significantly modify the accuracy of the state preparation. This is more clear looking at Fig. 12(c), where the same data are plotted but now using a logarithmic scale. There, it can be seen that although noise

limits the perfect fidelity in the state preparation that we were finding in the noiseless case, error rates of 2% still provide infidelities below 10^{-3} in a very short time, providing much better results than the equivalent adiabatic state preparations shown in the paper.

Figures 12(d)–12(f), on the other hand, show the same situation but now in the case of the coupling of dimers to prepare the ground state of a plaquette. In this case, the Hamiltonian quenched is $\hat{H}^{(2)}$ [cf. Eq. (B2)], with U again fixed to $U/t = 8$ and the variational parameters being $\tilde{t}$, the total length of the quench, and again the ramping time. In this case, three different quenches (three adiabatic ramps followed by three constant pulses) are able to generate the plaquette ground state with great accuracy. More remarkably, this case is significantly resistant to noise, providing very similar results independently of the amplitude of the noise [as shown in Fig. 12(f)]. This confirms that the intuition of the smoothness of the cost-function landscape stated above due to physical arguments is true, so we expect that this noise resilience will hold as further subsystems are variationally coupled.

APPENDIX E: IMPLEMENTING QUANTUM IMAGINARY-TIME EVOLUTION IN A PROGRAMMABLE SIMULATOR

QITE approximately solves the Wick-rotated Schrödinger equation in imaginary time $\tau \equiv iT$ to find an approximation of the ground state of a Hamiltonian $\hat{H}$. The equation

$$\frac{\partial}{\partial \tau} |\Psi(\tau)\rangle = -(\hat{H} - E_\tau) |\Psi(\tau)\rangle, \quad (\text{E1})$$

where $E_\tau = \langle \Psi(\tau) | \hat{H} | \Psi(\tau) \rangle$, is formally solved for an initial state $|\Psi_0\rangle$ as

$$|\Psi(\tau)\rangle = \frac{e^{-\tau \hat{H}} |\Psi_0\rangle}{\sqrt{\langle \Psi_0 | e^{-2\tau \hat{H}} | \Psi_0 \rangle}}. \quad (\text{E2})$$

In the eigenbasis of $\hat{H}$, $\{|\varphi_i\rangle\}$, the solution $|\Psi(\tau)\rangle$ reads

$$|\Psi(\tau)\rangle \propto c_0 |\varphi_0\rangle + \sum_{n>0} c_n e^{-(E_n - E_0)\tau} |\varphi_n\rangle, \quad (\text{E3})$$

where the E_i the eigenenergies, ordered in increasing value. Hence, from Eq. (E3), it is clear that $|\Psi(\tau)\rangle$ converges to the (nondegenerate) ground state $|\varphi_0\rangle$ of $\hat{H}$ in the limit $\tau \rightarrow \infty$.

Since the imaginary-time evolution is not unitary, obtaining Eq. (E1) with a quantum device requires us to approximate this action with a unitary operator. A possible way to do this involves approximating the exact ground

state with a parametrized trial state,

$$|\psi(\boldsymbol{\theta}(\tau))\rangle = \mathcal{U}(\boldsymbol{\theta}(\tau)) |\psi_0\rangle, \quad (\text{E4})$$

where $\boldsymbol{\theta} \in \mathbb{R}^d$ is a d -dimensional parameter vector that depends on the imaginary time. In particular, we will consider parametrized states generated by unitaries of the form

$$\mathcal{U}(\boldsymbol{\theta}(\tau)) = \prod_{\mu} e^{-i\theta_{\mu}(\tau)H_{\mu}}, \quad (\text{E5})$$

where the different H_{μ} are Hamiltonian terms that can be easily generated in the quantum simulator, such as those belonging to the gate set $\mathcal{G}$ in Eq. (5) for the case considered here, and the θ_{μ} are the elements of $\boldsymbol{\theta}$. With such a configuration, the variational quantum imaginary-time evolution (VarQITE) algorithm [87–89] maps the evolution of the quantum state $|\Psi\rangle$ to one of the vectors of parameters $\boldsymbol{\theta}$ using a variational method.

The application of McLachlan’s principle for this particular case, as described in Ref. [88], minimizes the distance between the exact imaginary-time wave function and the variational one, which is equivalent to the solution of the problem

$$\delta \left\| \left(\frac{\partial}{\partial \tau} + \hat{H} - E_{\tau} \right) |\psi(\boldsymbol{\theta}(\tau))\rangle \right\|. \quad (\text{E6})$$

Assuming $\boldsymbol{\theta}(\tau)$ to be real, Eq. (E6) becomes

$$g(\boldsymbol{\theta}(\tau)) \frac{d\boldsymbol{\theta}}{d\tau} = \mathbf{b}(\boldsymbol{\theta}(\tau)), \quad (\text{E7})$$

which is the projection of Eq. (E1) onto the variational manifold. In Eq. (E7), we have introduced the matrix $g = \text{Re}[G]$ as the real part of the quantum geometric tensor,

$$g_{\mu\nu}(\boldsymbol{\theta}) = \text{Re} \left[\langle \partial_{\mu} \psi(\boldsymbol{\theta}) | \partial_{\nu} \psi(\boldsymbol{\theta}) \rangle \right] - \text{Re} \left[\langle \partial_{\mu} \psi(\boldsymbol{\theta}) | \psi(\boldsymbol{\theta}) \rangle \langle \psi(\boldsymbol{\theta}) | \partial_{\nu} \psi(\boldsymbol{\theta}) \rangle \right], \quad (\text{E8})$$

where we have introduced the notation $\partial_{\mu} := \partial/\partial\theta_{\mu}$ and the evolution gradient $\mathbf{b}$:

$$b_{\mu}(\boldsymbol{\theta}) = -\text{Re} \left[\langle \partial_{\mu} \psi(\boldsymbol{\theta}) | H | \psi(\boldsymbol{\theta}) \rangle \right]. \quad (\text{E9})$$

We note that $b_{\mu}(\boldsymbol{\theta}) = -\partial_{\mu} E(\boldsymbol{\theta})/2$, i.e., $\mathbf{b}(\boldsymbol{\theta})$ is proportional to the gradient of the energy evaluated at $\boldsymbol{\theta}$.

If the parametrized state has enough expressibility (i.e., has the capability to accurately explore the relevant Hilbert space), Eq. (E1) is completely equivalent to Eq. (E7). Although in general this is not the case, Eq. (E7) still provides a good approximation to solve the real-time Schrödinger equation if the parametrized state is chosen

properly. The solution of the linear system of ODEs in Eq. (E7) involves a feedback loop between the classical and the quantum parts of the algorithm. In practice, Eq. (E7) is integrated numerically using an ODE solver. For example, a first-order Runge-Kutta method (or Euler method) with a time step $\Delta\tau$ leads to the following equivalent equation in the limit $\Delta\tau \rightarrow 0$:

$$g(\tau_n) \frac{\boldsymbol{\theta}(\tau_{n+1}) - \boldsymbol{\theta}(\tau_n)}{\Delta\tau} = \mathbf{b}(\tau_n), \quad (\text{E10})$$

where $\tau_n := n\Delta\tau$. Assuming knowledge of the parameters $\boldsymbol{\theta}(\tau_n)$ at step n , the above equation can be solved to yield the following update rule:

$$\boldsymbol{\theta}(\tau_{n+1}) = \boldsymbol{\theta}(\tau_n) + \Delta\tau g^+(\tau_n) \mathbf{b}(\tau_n), \quad (\text{E11})$$

where g^+ is the pseudoinverse of the metric tensor g (usually regularized by adding a small positive constant along the diagonal terms). Therefore, measuring the values of g and $\mathbf{b}$ at each step $\boldsymbol{\theta}(\tau_n)$ is enough to obtain the next set of parameters, $\boldsymbol{\theta}(\tau_{n+1})$.

Unfortunately, the measurement of both g and $\mathbf{b}$ following Eqs. (E8) and (E9) involves the measurement of real or imaginary parts of complicated objects as the number of parameters and the imaginary time-evolution increase. In a digital quantum device, this could be solved using controlled unitary operations [88]; however, in a cold-atom platform, it would be desirable to avoid this overhead. Although there are proposals to do so, such as in Ref. [121], the measurement of g and $\mathbf{b}$ would add an extra layer of complexity to the algorithm.

To avoid this overhead, and inspired by the nonvariational QITE algorithm in Ref. [86], we propose a way to solve Eq. (E1) iteratively for each time step $\Delta\tau$ using the variational approximation. If the state at τ_n is known, the state at τ_{n+1} can be obtained exactly, as

$$|\Psi(\tau_{n+1})\rangle = c(\tau_n) e^{-\Delta\tau \hat{H}} |\Psi(\tau_n)\rangle, \quad (\text{E12})$$

where $c(\tau_n) = 1/\|e^{-\Delta\tau \hat{H}} |\Psi(\tau_n)\rangle\|$ is a normalization constant. Then, taking $|\Psi_0\rangle = |\psi_0\rangle = |\psi(\tau_0)\rangle$ (i.e., the exact imaginary-time evolved state at $\tau = 0$ according to Eq. (E3) matches the parametrized quantum state when $\boldsymbol{\theta} = 0$) and considering the parametrized states as the ones in Eq. (E5), then Eqs. (E8) and (E9) become

$$\begin{aligned} g_{\mu\nu}(\boldsymbol{\theta}(\tau_0)) &= \text{Re} \left[\langle \psi_0 | \hat{H}_{\mu} \hat{H}_{\nu} | \psi_0 \rangle \right] \\ &\quad - \langle \psi_0 | \hat{H}_{\mu} | \psi_0 \rangle \langle \psi_0 | \hat{H}_{\nu} | \psi_0 \rangle, \\ b_{\mu}(\boldsymbol{\theta}(\tau_0)) &= \text{Im} \left[\langle \psi_0 | \hat{H}_{\mu} \hat{H} | \psi_0 \rangle \right], \end{aligned} \quad (\text{E13})$$

which can be measured using the methods described in Appendix C. Hence, from Eq. (E11), it is possible to obtain

the state at time τ_1 , $|\psi(\tau_1)\rangle$. Now, based on Eq. (E12), we consider this state to be the new initial state, so we map $|\psi(\tau_1)\rangle \rightarrow |\psi_0\rangle$ and measure the terms in Eq. (E13) over this state instead of $|\psi_0\rangle$. The application of the update rule in Eq. (E11) now gives us a new set of parameters that parametrize a quantum circuit generating the state $|\psi(\tau_2)\rangle$ from the state $|\psi(\tau_1)\rangle$. Applying this protocol iteratively, it is possible to obtain a variational approximation of the imaginary-time evolved quantum state up to τ_n , but always measuring objects of the form described in Eq. (E13).

1. Implementing the QLanczos algorithm using the data obtained with the QITE

Finally, to implementation of the QLanczos algorithm, it is necessary to measure the matrices $\mathbb{H}$ and $\mathbb{S}$, which read

$$\mathbb{H}_{\alpha,\beta} = \langle \Psi(\tau_\alpha) | \hat{H} | \Psi(\tau_\beta) \rangle, \quad (\text{E14})$$

$$\mathbb{S}_{\alpha,\beta} = \langle \Psi(\tau_\alpha) | \Psi(\tau_\beta) \rangle, \quad (\text{E15})$$

where $|\Psi(\tau_\alpha)\rangle = c_\alpha e^{-\alpha\Delta\tau\hat{H}} |\Psi_0\rangle$. To measure these matrices, one can always directly compute each matrix element using the variational approximation of $|\Psi(\tau_\alpha)\rangle$, $|\psi(\theta(\tau_\alpha))\rangle$, computing the absolute value of the term first and then its phase. A suitable way to obtain the absolute value would be to use the compute-uncompute method of Refs. [89,155]. This protocol computes the absolute value $|\langle\varphi|\psi\rangle|$, where $|\psi\rangle$ is prepared somehow and $|\varphi\rangle = \mathcal{U}|\varphi_0\rangle$, with $|\varphi_0\rangle$ being a product state in the occupation basis (terms of the form $|\langle\varphi|\hat{H}|\psi\rangle|$ could be computed identically by decomposing $\hat{H}$ as a linear combination of unitaries [156] and absorbing each unitary into $|\psi\rangle$). To do so, the compute-uncompute method is based on the application of a unitary $\mathcal{V}$ such as $|\langle\varphi_0|\mathcal{V}|\varphi\rangle| = 1$, so $\langle\varphi| = e^{i\phi} \langle\varphi_0|\mathcal{V}$. Then,

$$|\langle\varphi|\psi\rangle| = |\langle\varphi_0|\mathcal{V}|\psi\rangle|, \quad (\text{E16})$$

and now the projection over $\langle\varphi_0|$ can be done measuring in the occupation basis directly (since it is a product state in that basis). Regarding the operator $\mathcal{V}$, it can be implemented directly as the inverse of $\mathcal{U}$, $\mathcal{U}^\dagger$, by reverting all the signs of the unitaries and its order in the state preparation. However, variational strategies to recompile it with only positive signs can also be applied. On the other hand, once the absolute values $|\mathbb{H}_{\alpha,\beta}|$ and $|\mathbb{S}_{\alpha,\beta}|$ are measured, the estimation of its complex phases could be done following the algorithm described in Ref. [121].

However, in the main text we also introduce Eqs. (25) and (26) to approximately measure these matrices. To derive these approximations we follow the ideas introduced in Ref. [86]. First, let us note that the normalization

constant at step γ is

$$\frac{1}{c_\gamma^2} = \langle \Psi_0 | e^{-2\gamma\Delta\tau\hat{H}} | \Psi_0 \rangle. \quad (\text{E17})$$

Then, $\mathbb{S}_{\alpha,\beta}$ can be rewritten as

$$\begin{aligned} \mathbb{S}_{\alpha,\beta} &= \langle \Psi_0 | c_\alpha e^{-\alpha\Delta\tau\hat{H}} c_\beta e^{-\beta\Delta\tau\hat{H}} | \Psi_0 \rangle \\ &= c_\alpha c_\beta \langle \Psi_0 | e^{-(\alpha+\beta)\Delta\tau\hat{H}} | \Psi_0 \rangle = \frac{c_\alpha c_\beta}{c_{\frac{\alpha+\beta}{2}}^2} \end{aligned} \quad (\text{E18})$$

and the matrix elements of $\mathbb{H}_{\alpha,\beta}$ read

$$\begin{aligned} \mathbb{H}_{\alpha,\beta} &= \langle \Psi_0 | c_\alpha e^{-\alpha\Delta\tau\hat{H}} \hat{H} c_\beta e^{-\beta\Delta\tau\hat{H}} | \Psi_0 \rangle \\ &= c_\alpha c_\beta \langle \Psi_0 | e^{-\frac{\alpha+\beta}{2}\Delta\tau\hat{H}} \hat{H} e^{-\frac{\alpha+\beta}{2}\Delta\tau\hat{H}} | \Psi_0 \rangle \\ &= \frac{c_\alpha c_\beta}{c_{\frac{\alpha+\beta}{2}}^2} \langle \Psi_{\frac{\alpha+\beta}{2}} | \hat{H} | \Psi_{\frac{\alpha+\beta}{2}} \rangle = \mathbb{S}_{\alpha,\beta} \langle \Psi_{\frac{\alpha+\beta}{2}} | \hat{H} | \Psi_{\frac{\alpha+\beta}{2}} \rangle. \end{aligned} \quad (\text{E19})$$

Hence, all the matrix elements can be computed using the normalization constants and measurements of the energy. Finally, the normalization constants can be computed recursively noting that $c_0 = 1$ and, from Eq. (E17),

$$\begin{aligned} \frac{1}{c_{\gamma+1}^2} &= \langle \Psi_0 | e^{-2(\gamma+1)\Delta\tau\hat{H}} | \Psi_0 \rangle = \frac{\langle \Psi_\gamma | e^{-2\Delta\tau\hat{H}} | \Psi_\gamma \rangle}{c_\gamma^2} \\ &= \frac{1 - 2\Delta\tau \langle \Psi_\gamma | \hat{H} | \Psi_\gamma \rangle}{c_\gamma^2} + \mathcal{O}(\Delta\tau^2), \end{aligned} \quad (\text{E20})$$

where in the last line we have expanded the exponential up to first order in $\Delta\tau$.

-
- [1] D. Jaksch and P. Zoller, The cold atom Hubbard toolbox, *Ann. Phys.* **315**, 52 (2005), special Issue.
 - [2] M. Lewenstein, A. Sanpera, V. Ahufinger, B. Damski, A. Sen(De), and U. Sen, Ultracold atomic gases in optical lattices: Mimicking condensed matter physics and beyond, *Adv. Phys.* **56**, 243 (2007).
 - [3] C. Gross and I. Bloch, Quantum simulations with ultracold atoms in optical lattices, *Science* **357**, 995 (2017).
 - [4] F. Schäfer, T. Fukuhara, S. Sugawa, Y. Takasu, and Y. Takahashi, Tools for quantum simulation with ultracold atoms in optical lattices, *Nat. Rev. Phys.* **2**, 411 (2020).
 - [5] R. A. Hart, P. M. Duarte, T.-L. Yang, X. Liu, T. Paiva, E. Khatami, R. T. Scalettar, N. Trivedi, D. A. Huse, and R. G. Hulet, Observation of antiferromagnetic correlations in the Hubbard model with ultracold atoms, *Nature* **519**, 211 (2015).
 - [6] M. Boll, T. A. Hilker, G. Salomon, A. Omran, J. Nespolo, L. Pollet, I. Bloch, and C. Gross, Spin- and density-resolved microscopy of antiferromagnetic correlations in Fermi-Hubbard chains, *Science* **353**, 1257 (2016).

- [7] L. W. Cheuk, M. A. Nichols, K. R. Lawrence, M. Okan, H. Zhang, E. Khatami, N. Trivedi, T. Paiva, M. Rigol, and M. W. Zwierlein, Observation of spatial charge and spin correlations in the 2D Fermi-Hubbard model, *Science* **353**, 1260 (2016).
- [8] A. Mazurenko, C. S. Chiu, G. Ji, M. F. Parsons, M. Kanász-Nagy, R. Schmidt, F. Grusdt, E. Demler, D. Greif, and M. Greiner, A cold-atom Fermi-Hubbard antiferromagnet, *Nature* **545**, 462 (2017).
- [9] M. Xu, L. H. Kendrick, A. Kale, Y. Gang, G. Ji, R. T. Scalettar, M. Lebrat, and M. Greiner, Frustration- and doping-induced magnetism in a Fermi-Hubbard simulator, *Nature* **620**, 971 (2023).
- [10] H.-J. Shao, Y.-X. Wang, D.-Z. Zhu, Y.-S. Zhu, H.-N. Sun, S.-Y. Chen, C. Zhang, Z.-J. Fan, Y. Deng, X.-C. Yao, Y.-A. Chen, and J.-W. Pan, Antiferromagnetic phase transition in a 3D fermionic Hubbard model, *Nature* **632**, 267 (2024).
- [11] C. S. Chiu, G. Ji, A. Bohrdt, M. Xu, M. Knap, E. Demler, F. Grusdt, M. Greiner, and D. Greif, String patterns in the doped Hubbard model, *Science* **365**, 251 (2019).
- [12] D. Bourgund, T. Chalopin, P. Bojović, H. Schlömer, S. Wang, T. Franz, S. Hirthe, A. Bohrdt, F. Grusdt, I. Bloch, and T. A. Hilker, Formation of stripes in a mixed-dimensional cold-atom Fermi-Hubbard system, *Nature* **637**, 57 (2025).
- [13] P. Sompet, S. Hirthe, D. Bourgund, T. Chalopin, J. Bibo, J. Koepsell, P. Bojović, R. Verresen, F. Pollmann, G. Salomon, C. Gross, T. A. Hilker, and I. Bloch, Realizing the symmetry-protected Haldane phase in Fermi-Hubbard ladders, *Nature* **606**, 484 (2022).
- [14] S. Hirthe, T. Chalopin, D. Bourgund, P. Bojović, A. Bohrdt, E. Demler, F. Grusdt, I. Bloch, and T. A. Hilker, Magnetically mediated hole pairing in fermionic ladders of ultracold atoms, *Nature* **613**, 463 (2023).
- [15] T. Hartke, B. Oreg, C. Turnbaugh, N. Jia, and M. Zwierlein, Direct observation of nonlocal fermion pairing in an attractive Fermi-Hubbard gas, *Science* **381**, 82 (2023).
- [16] M. Schreiber, S. S. Hodgman, P. Bordia, H. P. Lüschen, M. H. Fischer, R. Vosk, E. Altman, U. Schneider, and I. Bloch, Observation of many-body localization of interacting fermions in a quasirandom optical lattice, *Science* **349**, 842 (2015).
- [17] M. A. Nichols, L. W. Cheuk, M. Okan, T. R. Hartke, E. Mendez, T. Senthil, E. Khatami, H. Zhang, and M. W. Zwierlein, Spin transport in a Mott insulator of ultracold fermions, *Science* **363**, 383 (2019).
- [18] E. Guardado-Sanchez, A. Morningstar, B. M. Spar, P. T. Brown, D. A. Huse, and W. S. Bakr, Subdiffusion and heat transport in a tilted two-dimensional Fermi-Hubbard system, *Phys. Rev. X* **10**, 011042 (2020).
- [19] S. Scherg, T. Kohlert, P. Sala, F. Pollmann, B. Hebbe Madhusudhana, I. Bloch, and M. Aidelsburger, Observing non-ergodicity due to kinetic constraints in tilted Fermi-Hubbard chains, *Nat. Commun.* **12**, 4490 (2021).
- [20] M. C. Bañuls, R. Blatt, J. Catani, A. Celi, J. I. Cirac, M. Dalmonte, L. Fallani, K. Jansen, M. Lewenstein, S. Montangero, C. A. Muschik, B. Reznik, E. Rico, L. Tagliacozzo, K. Van Acoleyen, F. Verstraete, U.-J. Wiese, M. Wingate, J. Zakrzewski, and P. Zoller, Simulating lattice gauge theories within quantum technologies, *Eur. Phys. J. D* **74**, 165 (2020).
- [21] M. Aidelsburger *et al.*, Cold atoms meet lattice gauge theory, *Philos. Trans. R. Soc. A* **380**, 20210064 (2022).
- [22] A. Di Meglio *et al.*, Quantum computing for high-energy physics: State of the art and challenges, *PRX Quantum* **5**, 037001 (2024).
- [23] F. Arute *et al.*, Google AI Quantum and Collaborators, Hartree-Fock on a superconducting qubit quantum computer, *Science* **369**, 1084 (2020).
- [24] F. Arute *et al.*, Observation of separated dynamics of charge and spin in the Fermi-Hubbard model, *ArXiv:2010.07965*.
- [25] S. Stanisic, J. L. Bosse, F. M. Gabbetta, R. A. Santos, W. Mruczkiewicz, T. E. O'Brien, E. Ostby, and A. Montanaro, Observing ground-state properties of the Fermi-Hubbard model using a scalable algorithm on a quantum computer, *Nat. Commun.* **13**, 5743 (2022).
- [26] R. N. Tazhigulov, S.-N. Sun, R. Haghshenas, H. Zhai, A. T. Tan, N. C. Rubin, R. Babbush, A. J. Minnich, and G. K.-L. Chan, Simulating models of challenging correlated molecules and materials on the Sycamore quantum processor, *PRX Quantum* **3**, 040318 (2022).
- [27] K. Hémerly, K. Ghanem, E. Crane, S. L. Campbell, J. M. Dreiling, C. Figgatt, C. Foltz, J. P. Gaebler, J. Johansen, M. Mills, S. A. Moses, J. M. Pino, A. Ransford, M. Rowe, P. Siegfried, R. P. Stutz, H. Dreyer, A. Schuckert, and R. Nigmatullin, Measuring the Loschmidt amplitude for finite-energy properties of the Fermi-Hubbard model on an ion-trap quantum computer, *PRX Quantum* **5**, 030323 (2024).
- [28] L. Clinton, T. Cubitt, B. Flynn, F. M. Gabbetta, J. Klassen, A. Montanaro, S. Piddock, R. A. Santos, and E. Sheridan, Towards near-term quantum simulation of materials, *Nat. Commun.* **15**, 211 (2024).
- [29] J. Robledo-Moreno, M. Motta, H. Haas, A. Javadi-Abhari, P. Jurcevic, W. Kirby, S. Martiel, K. Sharma, S. Sharma, T. Shirakawa, I. Sitdikov, R.-Y. Sun, K. J. Sung, M. Takita, M. C. Tran, S. Yunoki, and A. Mezzacapo, Chemistry beyond exact solutions on a quantum-centric supercomputer, *Sci. Adv.* **11**, eadu9991 (2025).
- [30] S. J. Evered, M. Kalinowski, A. A. Geim, T. Manovitz, D. Bluvstein, S. H. Li, N. Maskara, H. Zhou, S. Ebadi, M. Xu, J. Campo, M. Cain, S. Ostermann, S. F. Yelin, S. Sachdev, M. Greiner, V. Vuletić, and M. D. Lukin, Probing topological matter and fermion dynamics on a neutral-atom quantum computer, *ArXiv:2501.18554*.
- [31] D. S. Abrams and S. Lloyd, Simulation of many-body Fermi systems on a universal quantum computer, *Phys. Rev. Lett.* **79**, 2586 (1997).
- [32] G. Ortiz, J. E. Gubernatis, E. Knill, and R. Laflamme, Quantum algorithms for fermionic simulations, *Phys. Rev. A* **64**, 022319 (2001).
- [33] S. B. Bravyi and A. Y. Kitaev, Fermionic quantum computation, *Ann. Phys.* **298**, 210 (2002).
- [34] R. C. Ball, Fermions without fermion fields, *Phys. Rev. Lett.* **95**, 176407 (2005).
- [35] F. Verstraete and J. I. Cirac, Mapping local Hamiltonians of fermions to local Hamiltonians of spins, *J. Stat. Mech.: Theory and Exp.* **2005**, P09012 (2005).

- [36] J. D. Whitfield, J. Biamonte, and A. Aspuru-Guzik, Simulation of electronic structure Hamiltonians using quantum computers, *Mol. Phys.* **109**, 735 (2011).
- [37] J. D. Whitfield, V. c. v. Havlíček, and M. Troyer, Local spin operators for fermion simulations, *Phys. Rev. A* **94**, 030301 (2016).
- [38] J. Preskill, Quantum computing in the NISQ era and beyond, *Quantum* **2**, 79 (2018).
- [39] A. J. Daley, I. Bloch, C. Kokail, S. Flannigan, N. Pearson, M. Troyer, and P. Zoller, Practical quantum advantage in quantum simulation, *Nature* **607**, 667 (2022).
- [40] S. Flannigan, N. Pearson, G. H. Low, A. Buyskikh, I. Bloch, P. Zoller, M. Troyer, and A. J. Daley, Propagation of errors and quantitative quantum simulation with quantum advantage, *Quantum Sci. Technol.* **7**, 045025 (2022).
- [41] R. Trivedi, A. Franco Rubio, and J. I. Cirac, Quantum advantage and stability to errors in analogue quantum simulators, *Nat. Commun.* **15**, 6507 (2024).
- [42] B. F. Schiffer, A. F. Rubio, R. Trivedi, and J. I. Cirac, The quantum adiabatic algorithm suppresses the proliferation of errors, *ArXiv:2404.15397*.
- [43] V. Kashyap, G. Styliaris, S. Mouradian, J. I. Cirac, and R. Trivedi, Accuracy guarantees and quantum advantage in analog open quantum simulation with and without noise, *Phys. Rev. X* **15**, 021017 (2025).
- [44] B. Yang, H. Sun, R. Ott, H. Y. Wang, T. V. Zache, J. C. Halimeh, Z. S. Yuan, P. Hauke, and J. W. Pan, Observation of gauge invariance in a 71-site Bose-Hubbard quantum simulator, *Nature* **587**, 392 (2020).
- [45] A. L. Shaw, Z. Chen, J. Choi, D. K. Mark, P. Scholl, R. Finkelstein, A. Elben, S. Choi, and M. Endres, Benchmarking highly entangled states on a 60-atom analogue quantum simulator, *Nature* **628**, 71 (2024).
- [46] D. Adler, D. Wei, M. Will, K. Srakaew, S. Agrawal, P. Weckesser, R. Moessner, F. Pollmann, I. Bloch, and J. Zeiher, Observation of Hilbert space fragmentation and fractonic excitations in 2D, *Nature* **636**, 80 (2024).
- [47] T. I. Andersen *et al.*, Thermalization and criticality on an analogue-digital quantum simulator, *Nature* **638**, 79 (2025).
- [48] M. Qin, T. Schäfer, S. Andergassen, P. Corboz, and E. Gull, The Hubbard model: A computational perspective, *Annu. Rev. Condens. Matter Phys.* **13**, 275 (2022).
- [49] M. Qin, C.-M. Chung, H. Shi, E. Vitali, C. Hubig, U. Schollwöck, S. R. White, and S. Zhang, (Simons Collaboration on the Many-Electron Problem), Absence of superconductivity in the pure two-dimensional Hubbard model, *Phys. Rev. X* **10**, 031016 (2020).
- [50] H. Xu, C.-M. Chung, M. Qin, U. Schollwöck, S. R. White, and S. Zhang, Coexistence of superconductivity with partially filled stripes in the Hubbard model, *Science* **384**, eadh7691 (2024).
- [51] H.-N. Dai, B. Yang, A. Reingruber, X.-F. Xu, X. Jiang, Y.-A. Chen, Z.-S. Yuan, and J.-W. Pan, Generation and detection of atomic spin entanglement in optical lattices, *Nat. Phys.* **12**, 783 (2016).
- [52] X. Qiu, J. Zou, X. Qi, and X. Li, Precise programmable quantum simulations with optical lattices, *Npj Quantum Inf.* **6**, 87 (2020).
- [53] B. Yang, H. Sun, C.-J. Huang, H.-Y. Wang, Y. Deng, H.-N. Dai, Z.-S. Yuan, and J.-W. Pan, Cooling and entangling ultracold atoms in optical lattices, *Science* **369**, 550 (2020).
- [54] W.-Y. Zhang *et al.*, Scalable multipartite entanglement created by spin exchange in an optical lattice, *Phys. Rev. Lett.* **131**, 073401 (2023).
- [55] T. Chalopin, P. Bojović, D. Bourgund, S. Wang, T. Franz, I. Bloch, and T. Hilker, Optical superlattice for engineering Hubbard couplings in quantum simulation, *Phys. Rev. Lett.* **134**, 053402 (2025).
- [56] D. Wei, D. Adler, K. Srakaew, S. Agrawal, P. Weckesser, I. Bloch, and J. Zeiher, Observation of brane parity order in programmable optical lattices, *Phys. Rev. X* **13**, 021042 (2023).
- [57] A. Impertro, S. Karch, J. F. Wienand, S. Huh, C. Schweizer, I. Bloch, and M. Aidelsburger, Local readout and control of current and kinetic energy operators in optical lattices, *Phys. Rev. Lett.* **133**, 063401 (2024).
- [58] D. González-Cuadra, D. Bluvstein, M. Kalinowski, R. Kaubruegger, N. Maskara, P. Naldesi, T. V. Zache, A. M. Kaufman, M. D. Lukin, H. Pichler, B. Vermersch, J. Ye, and P. Zoller, Fermionic quantum processing with programmable neutral atom arrays, *Proc. Natl. Acad. Sci.* **120**, e2304294120 (2023).
- [59] T. V. Zache, D. González-Cuadra, and P. Zoller, Fermion-qudit quantum processors for simulating lattice gauge theories with matter, *Quantum* **7**, 1140 (2023).
- [60] Q. Li, C. Mukhopadhyay, and A. Bayat, Fermionic simulators for enhanced scalability of variational quantum simulation, *Phys. Rev. Res.* **5**, 043175 (2023).
- [61] F. Gkritis, D. Dux, J. Zhang, N. Jain, C. Gogolin, and P. M. Preiss, Simulating chemistry with fermionic optical superlattices, *PRX Quantum* **6**, 010318 (2025).
- [62] A. Schuckert, E. Crane, A. V. Gorshkov, M. Hafezi, and M. J. Gullans, Fault-tolerant fermionic quantum computing, *ArXiv:2411.08955v2*.
- [63] R. Ott, D. González-Cuadra, T. V. Zache, P. Zoller, A. M. Kaufman, and H. Pichler, Error-corrected fermionic quantum processors with neutral atoms, *ArXiv:2412.16081*.
- [64] C. Kokail, C. Maier, R. van Bijnen, T. Brydges, M. K. Joshi, P. Jurcevic, C. A. Muschik, P. Silvi, R. Blatt, C. F. Roos, and P. Zoller, Self-verifying variational quantum simulation of lattice models, *Nature* **569**, 355 (2019).
- [65] C. Monroe, W. C. Campbell, L.-M. Duan, Z.-X. Gong, A. V. Gorshkov, P. W. Hess, R. Islam, K. Kim, N. M. Linke, G. Pagano, P. Richerme, C. Senko, and N. Y. Yao, Programmable quantum simulations of spin systems with trapped ions, *Rev. Mod. Phys.* **93**, 025001 (2021).
- [66] C. Joshi, F. Yang, and M. Mirhosseini, Resonance fluorescence of a chiral artificial atom, *Phys. Rev. X* **13**, 021039 (2023).
- [67] H. Labuhn, D. Barredo, S. Ravets, S. de Léséleuc, T. Macrì, T. Lahaye, and A. Browaeys, Tunable two-dimensional arrays of single Rydberg atoms for realizing quantum Ising models, *Nature* **534**, 667 (2016).
- [68] H. Bernien, S. Schwartz, A. Keesling, H. Levine, A. Omran, H. Pichler, S. Choi, A. S. Zibrov, M. Endres, M. Greiner, V. Vuletić, and M. D. Lukin, Probing many-body dynamics on a 51-atom quantum simulator, *Nature* **551**, 579 (2017).

- [69] A. Keesling, A. Omran, H. Levine, H. Bernien, H. Pichler, S. Choi, R. Samajdar, S. Schwartz, P. Silvi, S. Sachdev, P. Zoller, M. Endres, M. Greiner, V. Vuletić, and M. D. Lukin, Quantum Kibble-Zurek mechanism and critical dynamics on a programmable rydberg simulator, *Nature* **568**, 207 (2019).
- [70] S. de Léséleuc, V. Lienhard, P. Scholl, D. Barredo, S. Weber, N. Lang, H. P. Büchler, T. Lahaye, and A. Browaeys, Observation of a symmetry-protected topological phase of interacting bosons with Rydberg atoms, *Science* **365**, 775 (2019).
- [71] S. Ebadi, T. T. Wang, H. Levine, A. Keesling, G. Semeghini, A. Omran, D. Bluvstein, R. Samajdar, H. Pichler, W. W. Ho, S. Choi, S. Sachdev, M. Greiner, V. Vuletić, and M. D. Lukin, Quantum phases of matter on a 256-atom programmable quantum simulator, *Nature* **595**, 227 (2021).
- [72] P. Scholl, M. Schuler, H. J. Williams, A. A. Eberharter, D. Barredo, K.-N. Schymik, V. Lienhard, L.-P. Henry, T. C. Lang, T. Lahaye, A. M. Läuchli, and A. Browaeys, Quantum simulation of 2D antiferromagnets with hundreds of Rydberg atoms, *Nature* **595**, 233 (2021).
- [73] D. Bluvstein, A. Omran, H. Levine, A. Keesling, G. Semeghini, S. Ebadi, T. T. Wang, A. A. Michailidis, N. Maskara, W. W. Ho, S. Choi, M. Serbyn, M. Greiner, V. Vuletić, and M. D. Lukin, Controlling quantum many-body dynamics in driven Rydberg atom arrays, *Science* **371**, 1355 (2021).
- [74] G. Semeghini, H. Levine, A. Keesling, S. Ebadi, T. T. Wang, D. Bluvstein, R. Verresen, H. Pichler, M. Kalinowski, R. Samajdar, A. Omran, S. Sachdev, A. Vishwanath, M. Greiner, V. Vuletić, and M. D. Lukin, Probing topological spin liquids on a programmable quantum simulator, *Science* **374**, 1242 (2021).
- [75] P. Scholl, H. J. Williams, G. Bornet, F. Wallner, D. Barredo, L. Henriot, A. Signoles, C. Hainaut, T. Franz, S. Geier, A. Tebben, A. Salzinger, G. Zürn, T. Lahaye, M. Weidemüller, and A. Browaeys, Microwave engineering of programmable XXZ Hamiltonians in arrays of Rydberg atoms, *PRX Quantum* **3**, 020303 (2022).
- [76] T. Manovitz, S. H. Li, S. Ebadi, R. Samajdar, A. A. Geim, S. J. Evered, D. Bluvstein, H. Zhou, N. U. Köylüoğlu, J. Feldmeier, P. E. Dolgirev, N. Maskara, M. Kalinowski, S. Sachdev, D. A. Huse, M. Greiner, V. Vuletić, and M. D. Lukin, Quantum coarsening and collective dynamics on a programmable quantum simulator, *Nature* **638**, 86 (2025).
- [77] A. Lukin, B. F. Schiffer, B. Braverman, S. H. Cantu, F. Huber, A. Bylinskii, J. Amato-Grill, N. Maskara, M. Cain, D. S. Wild, R. Samajdar, and M. D. Lukin, Quantum quench dynamics as a shortcut to adiabaticity, *ArXiv:2405.21019*.
- [78] D. Gonzalez-Cuadra, M. Hamdan, T. V. Zache, B. Braverman, M. Kornjaca, A. Lukin, S. H. Cantu, F. Liu, S.-T. Wang, A. Keesling, M. D. Lukin, P. Zoller, and A. Bylinskii, Observation of string breaking on a $(2 + 1)$ D Rydberg quantum simulator, *Nature* **642**, 321 (2025).
- [79] M. Cerezo, A. Arrasmith, R. Babbush, S. C. Benjamin, S. Endo, K. Fujii, J. R. McClean, K. Mitarai, X. Yuan, L. Cincio, and P. J. Coles, Variational quantum algorithms, *Nat. Phys. Rev.* **3**, 625 (2021).
- [80] A. Peruzzo, J. McClean, P. Shadbolt, M.-H. Yung, X.-Q. Zhou, P. J. Love, A. Aspuru-Guzik, and J. L. O'Brien, A variational eigenvalue solver on a photonic quantum processor, *Nat. Commun.* **5**, 4213 (2014).
- [81] I. D. Kivlichan, J. McClean, N. Wiebe, C. Gidney, A. Aspuru-Guzik, G. K. L. Chan, and R. Babbush, Quantum simulation of electronic structure with linear depth and connectivity, *Phys. Rev. Lett.* **120**, 110501 (2018).
- [82] H. R. Grimsley, S. E. Economou, E. Barnes, and N. J. Mayhall, An adaptive variational algorithm for exact molecular simulations on a quantum computer, *Nat. Commun.* **10**, 1 (2019).
- [83] H. L. Tang, V. O. Shkolnikov, G. S. Barron, H. R. Grimsley, N. J. Mayhall, E. Barnes, and S. E. Economou, Qubit-ADAPT-VQE: An adaptive algorithm for constructing hardware-efficient ansätze on a quantum processor, *PRX Quantum* **2**, 020310 (2021).
- [84] T. Takeshita, N. C. Rubin, Z. Jiang, E. Lee, R. Babbush, and J. R. McClean, Increasing the representation accuracy of quantum simulations of chemistry without extra quantum resources, *Phys. Rev. X* **10**, 011004 (2020).
- [85] W. J. Huggins, J. R. McClean, N. C. Rubin, Z. Jiang, N. Wiebe, K. B. Whaley, and R. Babbush, Efficient and noise resilient measurements for quantum chemistry on near-term quantum computers, *Npj Quantum Inf.* **7**, 23 (2021).
- [86] M. Motta, C. Sun, A. T. Tan, M. J. O'Rourke, E. Ye, A. J. Minnich, F. G. Brandao, and G. K.-L. Chan, Determining eigenstates and thermal states on a quantum computer using quantum imaginary time evolution, *Nat. Phys.* **16**, 205 (2020).
- [87] S. McArdle, T. Jones, S. Endo, Y. Li, S. C. Benjamin, and X. Yuan, Variational ansatz-based quantum simulation of imaginary time evolution, *npj Quantum Inf.* **5**, 75 (2019).
- [88] X. Yuan, S. Endo, Q. Zhao, Y. Li, and S. C. Benjamin, Theory of variational quantum simulation, *Quantum* **3**, 191 (2019).
- [89] J. Gacon, J. Nys, R. Rossi, S. Woerner, and G. Carleo, Variational quantum time evolution without the quantum geometric tensor, *Phys. Rev. Res.* **6**, 013143 (2024).
- [90] A. M. Kaufman and K.-K. Ni, Quantum science with optical tweezer arrays of ultracold atoms and molecules, *Nat. Phys.* **17**, 1324 (2021).
- [91] A. W. Young, W. J. Eckner, N. Schine, A. M. Childs, and A. M. Kaufman, Tweezer-programmable 2D quantum walks in a Hubbard-regime lattice, *Science* **377**, 885 (2022).
- [92] Z. Z. Yan, B. M. Spar, M. L. Prichard, S. Chi, H.-T. Wei, E. Ibarra-García-Padilla, K. R. A. Hazzard, and W. S. Bakr, Two-dimensional programmable tweezer arrays of fermions, *Phys. Rev. Lett.* **129**, 123201 (2022).
- [93] R. Tao, M. Ammenwerth, F. Gyger, I. Bloch, and J. Zeiher, High-fidelity detection of large-scale atom arrays in an optical lattice, *Phys. Rev. Lett.* **133**, 013401 (2024).
- [94] P. Rabl, A. J. Daley, P. O. Fedichev, J. I. Cirac, and P. Zoller, Defect-suppressed atomic crystals in an optical lattice, *Phys. Rev. Lett.* **91**, 110403 (2003).
- [95] A. Griessner, A. J. Daley, S. R. Clark, D. Jaksch, and P. Zoller, Dissipative dynamics of atomic Hubbard models coupled to a phonon bath: Dark state cooling of atoms

- within a Bloch band of an optical lattice, *New J. Phys.* **9**, 44 (2007).
- [96] M. Popp, J.-J. Garcia-Ripoll, K. G. Vollbrecht, and J. I. Cirac, Ground-state cooling of atoms in optical lattices, *Phys. Rev. A* **74**, 013622 (2006).
- [97] W. S. Bakr, P. M. Preiss, M. E. Tai, R. Ma, J. Simon, and M. Greiner, Orbital excitation blockade and algorithmic cooling in quantum gases, *Nature* **480**, 500 (2011).
- [98] M. Xu, L. H. Kendrick, A. Kale, Y. Gang, C. Feng, S. Zhang, A. W. Young, M. Lebrat, and M. Greiner, A neutral-atom Hubbard quantum simulator in the cryogenic regime, *Nature* **642**, 909 (2025).
- [99] B. M. Spar, E. Guardado-Sanchez, S. Chi, Z. Z. Yan, and W. S. Bakr, Realization of a Fermi-Hubbard optical tweezer array, *Phys. Rev. Lett.* **128**, 223202 (2022).
- [100] S. Nascimbène, Y.-A. Chen, M. Atala, M. Aidelsburger, S. Trotzky, B. Paredes, and I. Bloch, Experimental realization of plaquette resonating valence-bond states with ultracold atoms in optical superlattices, *Phys. Rev. Lett.* **108**, 205301 (2012).
- [101] S. Trebst, U. Schollwöck, M. Troyer, and P. Zoller, d -wave resonating valence bond states of fermionic atoms in optical lattices, *Phys. Rev. Lett.* **96**, 250402 (2006).
- [102] B. Paredes and I. Bloch, Minimum instances of topological matter in an optical plaquette, *Phys. Rev. A* **77**, 023603 (2008).
- [103] A. M. Rey, R. Sensarma, S. Fölling, M. Greiner, E. Demler, and M. D. Lukin, Controlled preparation and detection of d -wave superfluidity in two-dimensional optical superlattices, *Europhys. Lett.* **87**, 60001 (2009).
- [104] M. Lubasch *et al.*, *Phys. Rev. Lett.* **107**, 165301 (2011).
- [105] W. S. Bakr, J. I. Gillen, A. Peng, S. Fölling, and M. Greiner, A quantum gas microscope for detecting single atoms in a Hubbard-regime optical lattice, *Nature* **462**, 74 (2009).
- [106] J. F. Sherson, C. Weitenberg, M. Endres, M. Cheneau, I. Bloch, and S. Kuhr, Single-atom-resolved fluorescence imaging of an atomic Mott insulator, *Nature* **467**, 68 (2010).
- [107] C. Gross and W. S. Bakr, Quantum gas microscopy for single atom and spin detection, *Nat. Phys.* **17**, 1316 (2021).
- [108] D. K. Mark, H.-Y. Hu, J. Kwan, C. Kokail, S. Choi, and S. F. Yelin, Efficiently measuring d -wave pairing and beyond in quantum gas microscopes, *ArXiv:2412.13186*.
- [109] T. Chalopin, P. Bojović, D. Bourgund, S. Wang, T. Franz, I. Bloch, and T. Hilker, Optical superlattice for engineering Hubbard couplings in quantum simulation, *Phys. Rev. Lett.* **134**, 053402 (2025).
- [110] L. Su, A. Douglas, M. Szurek, A. H. Hébert, A. Krahn, R. Groth, G. A. Phelps, O. Marković, and M. Greiner, Fast single atom imaging for optical lattice arrays, *Nat. Commun.* **16**, 1017 (2025).
- [111] One quantum gas microscope measurement is required for the interaction term. At most four measurements are necessary for all tunneling terms in a lattice, following Ref. [57] (although in translationally invariant systems this could be reduced). This results in five measurements needed to compute $\langle \hat{H} \rangle$, the energy of the target Hamiltonian. Assuming the parallel measurements of independent realizations in a region of interest, it is possible to perform approximately 50 measurements simultaneously [135]. Therefore, each experimental run yields about ten evaluations of $\langle \hat{H} \rangle$. Assuming that 200–300 evaluations are needed to obtain statistically significant results, this implies that 20–30 experimental runs are required for each final energy evaluation. If a total of 10^4 experiments are performed, this allows for approximately 300–500 final energy evaluations.
- [112] C. W. von Keyserlingk, T. Rakovszky, F. Pollmann, and S. L. Sondhi, Operator hydrodynamics, OTOCs, and entanglement growth in systems without conservation laws, *Phys. Rev. X* **8**, 021013 (2018).
- [113] L. Zhou, S.-T. Wang, S. Choi, H. Pichler, and M. D. Lukin, Quantum approximate optimization algorithm: Performance, mechanism, and implementation on near-term devices, *Phys. Rev. X* **10**, 021067 (2020).
- [114] R. Wiersema, C. Zhou, Y. de Sereville, J. F. Carrasquilla, Y. B. Kim, and H. Yuen, Exploring entanglement and optimization within the Hamiltonian variational ansatz, *PRX Quantum* **1**, 020319 (2020).
- [115] B.-X. Zheng, C.-M. Chung, P. Corboz, G. Ehlers, M.-P. Qin, R. M. Noack, H. Shi, S. R. White, S. Zhang, and G. K.-L. Chan, Stripe order in the underdoped region of the two-dimensional Hubbard model, *Science* **358**, 1155 (2017).
- [116] H.-C. Jiang and T. P. Devereaux, Superconductivity in the doped Hubbard model and its interplay with next-nearest hopping t' , *Science* **365**, 1424 (2019).
- [117] M. F. Parsons, A. Mazurenko, C. S. Chiu, G. Ji, D. Greif, and M. Greiner, Site-resolved measurement of the spin-correlation function in the Fermi-Hubbard model, *Science* **353**, 1253 (2016).
- [118] J. Koepsell, J. Vijayan, P. Sompet, F. Grusdt, T. A. Hilker, E. Demler, G. Salomon, I. Bloch, and C. Gross, Imaging magnetic polarons in the doped Fermi-Hubbard model, *Nature* **572**, 358 (2019).
- [119] B. Ponsioen, S. S. Chung, and P. Corboz, Period 4 stripe in the extended two-dimensional Hubbard model, *Phys. Rev. B* **100**, 195141 (2019).
- [120] M. Motta, W. Kirby, I. Liepuoniute, K. J. Sung, J. Cohn, A. Mezzacapo, K. Klymko, N. Nguyen, N. Yoshioka, and J. E. Rice, Subspace methods for electronic structure simulations on quantum computers, *Electron. Struct.* **6**, 013001 (2024).
- [121] Y. Yang, A. Christianen, M. C. Bañuls, D. S. Wild, and J. I. Cirac, Phase-sensitive quantum measurement without controlled operations, *Phys. Rev. Lett.* **132**, 220601 (2024).
- [122] D. Poulin and P. Wocjan, Preparing ground states of quantum many-body systems on a quantum computer, *Phys. Rev. Lett.* **102**, 130503 (2009).
- [123] Y. Ge, J. Tura, and J. I. Cirac, Faster ground state preparation and high-precision ground energy estimation with fewer qubits, *J. Math. Phys.* **60**, 022202 (2019).
- [124] L. Lin and Y. Tong, Near-optimal ground state preparation, *Quantum* **4**, 372 (2020).

- [125] S. Lu, M. C. Bañuls, and J. I. Cirac, Algorithms for quantum simulation at finite energies, *PRX Quantum* **2**, 020321 (2021).
- [126] R. D. Somma, Quantum eigenvalue estimation via time series analysis, *New J. Phys.* **21**, 123025 (2019).
- [127] T. E. O'Brien, B. Tarasinski, and B. M. Terhal, Quantum phase estimation of multiple eigenvalues for small-scale (noisy) experiments, *New J. Phys.* **21**, 023022 (2019).
- [128] L. Lin and Y. Tong, Heisenberg-limited ground-state energy estimation for early fault-tolerant quantum computers, *PRX Quantum* **3**, 010318 (2022).
- [129] Z. Ding and L. Lin, Even shorter quantum circuit for phase estimation on early fault-tolerant quantum computers with applications to ground-state energy estimation, *PRX Quantum* **4**, 020331 (2023).
- [130] G. Wang, D. S. França, R. Zhang, S. Zhu, and P. D. Johnson, Quantum algorithm for ground state energy estimation using circuit depth with exponentially improved dependence on precision, *Quantum* **7**, 1167 (2023).
- [131] C. Lanczos, An iteration method for the solution of the eigenvalue problem of linear differential and integral operators, *J. Res. Natl. Bur. Stand. B* **45**, 255 (1950).
- [132] S. Piccinelli, F. Tacchino, I. Tavernelli, and G. Carleo, Efficient calculation of Green's functions on quantum computers via simultaneous circuit perturbation, *ArXiv:2505.05563*.
- [133] M. Larocca, S. Thanasilp, S. Wang, K. Sharma, J. Biamonte, P. J. Coles, L. Cincio, J. R. McClean, Z. Holmes, and M. Cerezo, A review of barren plateaus in variational quantum computing, *Nature Rev. Phys.* **7**, 174 (2025).
- [134] A. A. Mele, G. B. Mbeng, G. E. Santoro, M. Collura, and P. Torta, Avoiding barren plateaus via transferability of smooth solutions in Hamiltonian variational ansatz, *Phys. Rev. A* **106**, L060401 (2022).
- [135] S. Karch, S. Bandyopadhyay, Z.-H. Sun, A. Impertro, S. Huh, I. P. Rodríguez, J. F. Wienand, W. Ketterle, M. Heyl, A. Polkovnikov, I. Bloch, and M. Aidelsburger, Probing quantum many-body dynamics using subsystem Loschmidt echos, *ArXiv:2501.16995*.
- [136] P. M. Preiss, R. Ma, M. E. Tai, J. Simon, and M. Greiner, Quantum gas microscopy with spin, atom-number, and multilayer readout, *Phys. Rev. A* **91**, 41602 (2015).
- [137] L. Asteria, H. P. Zahn, M. N. Kosch, K. Sengstock, and C. Weitenberg, Quantum gas magnifier for sub-lattice-resolved imaging of 3D quantum systems, *Nature* **599**, 571 (2021).
- [138] T. Legrand, F.-R. Winkelmann, W. Alt, D. Meschede, A. Alberti, and C. A. Weidner, Three-dimensional imaging of single atoms in an optical lattice via helical point-spread-function engineering, *Phys. Rev. A* **109**, 033304 (2024).
- [139] T. Chalopin, P. Bojović, S. Wang, T. Franz, A. Sinha, Z. Wang, D. Bourgund, J. Obermeyer, F. Grusdt, A. Bohrdt *et al.*, Probing the magnetic origin of the pseudogap using a Fermi-Hubbard quantum simulator, *ArXiv:2412.17801*.
- [140] P. Naldesi, A. Elben, A. Minguzzi, D. Clément, P. Zoller, and B. Vermersch, Fermionic correlation functions from randomized measurements in programmable atomic quantum devices, *Phys. Rev. Lett.* **131**, 060601 (2023).
- [141] M. Gluza and J. Eisert, Recovering quantum correlations in optical lattices from interaction quenches, *Phys. Rev. Lett.* **127**, 090503 (2021).
- [142] A. Zhao, N. C. Rubin, and A. Miyake, Fermionic partial tomography via classical shadows, *Phys. Rev. Lett.* **127**, 110504 (2021).
- [143] G. H. Low, Classical shadows of fermions with particle number symmetry, *ArXiv:2208.08964*.
- [144] J. Denzler, A. A. Mele, E. Derbyshire, T. Guaita, and J. Eisert, Learning fermionic correlations by evolving with random translationally invariant Hamiltonians, *Phys. Rev. Lett.* **133**, 240604 (2024).
- [145] M. C. Tran, D. K. Mark, W. W. Ho, and S. Choi, Measuring arbitrary physical properties in analog quantum simulation, *Phys. Rev. X* **13**, 011049 (2023).
- [146] M. Aidelsburger, S. Nascimbene, and N. Goldman, Artificial gauge fields in materials and engineered systems, *C. R. Phys.* **19**, 394 (2018).
- [147] L. Chomaz, I. Ferrier-Barbut, F. Ferlaino, B. Laburthe-Tolra, B. L. Lev, and T. Pfau, Dipolar physics: A review of experiments with magnetic quantum gases, *Rep. Prog. Phys.* **86**, 026401 (2022).
- [148] J. Argüello-Luengo, A. González-Tudela, and D. González-Cuadra, Tuning long-range fermion-mediated interactions in cold-atom quantum simulators, *Phys. Rev. Lett.* **129**, 083401 (2022).
- [149] L. Bilinskaya, *Phys. Rev. Res.* **6**, L042024 (2024).
- [150] J. Léonard, S. Kim, J. Kwan, P. Segura, F. Grusdt, C. Repellin, N. Goldman, and M. Greiner, Realization of a fractional quantum hall state with ultracold atoms, *Nature* **619**, 495 (2023).
- [151] C. Tabares, A. Muñoz de las Heras, L. Tagliacozzo, D. Porras, and A. González-Tudela, Variational quantum simulators based on waveguide QED, *Phys. Rev. Lett.* **131**, 073602 (2023).
- [152] M. Fishman, S. R. White, and E. M. Stoudenmire, The ITensor software library for tensor network calculations, *SciPost Phys. Codebases*, **4** (2022).
- [153] C. Tabares, Programming optical lattice fermionic quantum simulators, 2025, https://github.com/cristiantlopez/Programming_OpticalLattice_FermiHubbard_Quantum_Simulators
- [154] C. Tabares, Programming optical-lattice Fermi-Hubbard quantum simulators, 2025, <https://doi.org/10.5281/zenodo.16536686>
- [155] V. Havlíček, M. Troyer, and J. D. Whitfield, Operator locality in the quantum simulation of fermionic models, *Phys. Rev. A* **95**, 032332 (2017).
- [156] A. Childs and N. Wiebe, Hamiltonian simulation using linear combinations of unitary operations, *Quantum Inf. Comput.* **12**, 901 (2012).