

Correcting and Extending Trotterized Quantum Many-Body Dynamics

Gian Gentinetta^{1,2,*}, Friederike Metz^{1,2}, and Giuseppe Carleo^{1,2}

¹*Institute of Physics, École Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland*

²*Center for Quantum Science and Engineering, EPFL, CH-1015 Lausanne, Switzerland*

 (Received 9 April 2025; revised 1 July 2025; accepted 21 August 2025; published 24 September 2025)

A complex but important challenge in understanding quantum mechanical phenomena is the simulation of quantum many-body dynamics. Although quantum computers offer significant potential to accelerate these simulations, their practical application is currently limited by noise and restricted scalability. In this work, we address these problems by introducing a hybrid ansatz combining the strengths of quantum and classical computational methods. Using Trotterization, we propose to evolve an initial state on the quantum computer according to a simplified Hamiltonian, focusing on terms that are difficult to simulate classically. A classical model then corrects the simulation by including the terms omitted in the quantum circuit. While the classical ansatz is optimized during the time evolution, the quantum circuit has no variational parameters. Derivatives can thus be calculated purely classically, avoiding challenges arising in the optimization of parametrized quantum circuits. We demonstrate three applications of this hybrid method. First, our approach allows us to avoid SWAP gates in the quantum circuit by restricting the quantum part of the ansatz to hardware-efficient terms of the Hamiltonian. Second, we can mitigate errors arising from the Trotterization of the time-evolution unitary. Finally, we can extend the system size while keeping the number of qubits in the quantum circuit constant by including additional degrees of freedom in the classical ansatz.

DOI: [10.1103/1nqt-x5xh](https://doi.org/10.1103/1nqt-x5xh)

I. INTRODUCTION

Solving the time-dependent Schrödinger equation for quantum many-body systems is an important piece in the puzzle of understanding nature at a microscopic scale [1–6]. While analytical solutions quickly become unreachable as the number of particles increases, a plethora of computational methods are available to simulate the dynamics of such quantum systems up to a certain size [7–14]. However, as the Hilbert space scales exponentially in the number of particles, classical simulation methods are limited to relatively small system sizes. Quantum computers comprise a promising tool for this application, as the resources required for the simulation of quantum time evolution scale polynomially with the number of particles, in theory allowing for an advantage over classical algorithms [15–20].

In practice, quantum simulations using noisy intermediate-scale quantum (NISQ) devices [21] are

restricted by limited scale and the effects of noise [22–25]. As a consequence, the simulation of quantum dynamics through Trotterization of the time-evolution unitary [26,27] is effectively only approximate. Due to the limited coherence time, only a small number of Trotter steps can be implemented on digital quantum computers, leading to significant Trotter errors. Further, the restricted connectivity of near-term quantum devices prohibits direct implementation of the time evolution of nonlocal Hamiltonians without additional SWAP gates further increasing the circuit depth. Finally, the small number of qubits available on current devices constrains the system sizes that can be simulated.

In recent years, variational quantum algorithms have been proposed to address the problem of limited coherence time [28]. By keeping the circuit depth constant, longer simulation times can be reached compared to a Trotterized time evolution at the cost of optimizing circuit parameters [29–37]. The circuit ansatz can further be chosen to be hardware efficient, avoiding SWAP gates in the simulation of nonlocal Hamiltonians. The variational parameters are either updated using the time-dependent variational principle (TDVP) [29–32,38–41] or by minimizing a loss function at every time step [33–36]. These methods often rely on gradients computed via the parameter-shift rule [42,43], which prohibits

*Contact author: gian.gentinetta@epfl.ch

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.

back-propagation scaling [44]. While derivative-free optimizers exist, gradient-based approaches are more commonly used in practice. Other notable classical-assisted quantum simulation approaches developed for near-term devices include (variational) fast-forwarding [45,46], subspace methods [47,48], and adaptive Trotterization [49,50].

On the other hand, to overcome the restrictions imposed by the limited number of available qubits on near-term devices, a range of quantum-classical hybrid algorithms has been proposed to split a large quantum system into smaller partitions [51–55] for applications in ground-state problems [56–66] and, more recently, also for dynamics [35,67]. Crucially, the quantum circuits for the individual partitions remain parametrized and hence the challenges with computing derivatives remain. This is also the case for another class of hybrid algorithms, where a classical ansatz is combined with a parametrized quantum circuit to reach lower energies in discrete [68,69] or continuous [70] space ground-state problems.

In contrast, we propose a quantum-classical hybrid algorithm for the simulation of quantum dynamics that requires no optimization of parameters on the quantum circuit. Instead, we use Trotterized time evolution according to a simplified Hamiltonian containing terms that are difficult to simulate classically but can be efficiently implemented on the hardware. We then employ an optimizable classical ansatz to correct for the errors arising from the Trotterization as well as from the simplification of the Hamiltonian. As the quantum circuit is no longer parametrized, any derivatives can be computed purely classically using back-propagation. In fact, we show that all relevant quantities required for the optimization of the *classically corrected quantum dynamics (CQD)* ansatz can

be obtained by sampling the time-evolved quantum circuit in different bases and evaluating the classical part of the ansatz at those samples.

The remainder of the paper is structured as follows. In Sec. II, we define the ansatz, show how expectation values are computed, and derive the equations of motion for the classical parameter updates. In Sec. III, we showcase three applications of the method, demonstrating how the hybrid ansatz allows us to (i) correct Trotter errors [Sec. III A], (ii) avoid the use of SWAP gates by evolving with a hardware-efficient approximation of the Hamiltonian [Sec. III B], and (iii) extend the system size by treating additional degrees of freedom purely classically [Sec. III C]. Finally, in Sec. IV, we discuss the results and provide an outlook with regard to possible future applications of the method.

II. METHODS

Our goal is to simulate the time evolution of an initial state $|\psi_0\rangle$ with respect to a time-independent Hamiltonian H . Ideally, we want to evolve the quantum state directly with H on the quantum device, i.e., $|\psi^q(t)\rangle = e^{-iHt} |\psi_0\rangle$. However, consider the situation in which the time evolution on the hardware can only be simulated with an approximate Hamiltonian $\tilde{H}$. This problem naturally occurs when, e.g., the time-evolution unitary is Trotterized. In these cases, we propose to use a classical parametrized function $\psi_{\theta(t)}^c(z)$ to correct the dynamics (see Fig. 1) and optimize it using an extended version of the TDVP [41]. Specifically, we sample the time-evolved quantum state at incremental time steps to obtain the appropriate equations of motion for the parameters $\theta(t)$, which are then updated accordingly.

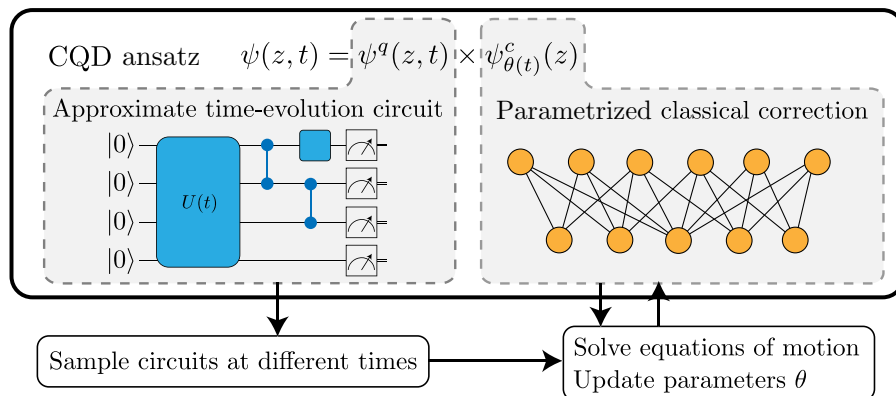


FIG. 1. A sketch of the classically corrected quantum dynamics (CQD) ansatz. In order to evolve the ansatz in time according to a Hamiltonian H , a quantum circuit (on the left) is evolved with an approximate time-evolution unitary $U(t)$. At every time step, the circuit is measured in multiple bases given by the Pauli decomposition of H and the effective Hamiltonian $\tilde{H}$ underlying $U(t)$. Those samples, together with the classical ansatz (on the right) are used to obtain the equations of motion that are integrated in order to update the classical parameters θ iteratively.

A. Hybrid ansatz

We define the Classically Corrected Quantum Dynamics (CQD) ansatz at time t in the computational basis spanned by bit strings z as

$$\psi_{\theta(t)}(t, z) = \langle z | \psi^q(t) \rangle \psi_{\theta(t)}^c(z) = \psi^q(t, z) \psi_{\theta(t)}^c(z), \quad (1)$$

where $|\psi^q(t)\rangle = U(t) |\psi_0\rangle$ is a quantum state implemented as a quantum circuit, with $U(t)$ a time-evolution unitary to be specified later, and ψ^c is the classical correction, such as a mean-field, Jastrow, or a neural-network ansatz. Importantly, the classical contribution to the wave function is parametrized with time-dependent parameters $\theta(t)$, while the time dependence of the quantum contribution is given explicitly through a deterministic time evolution of the initial state. Thus, the quantum circuit contains no optimizable parameters. Note that, in general, the hybrid wave function $\psi_{\theta(t)}(t, z)$ is not required to be normalized.

We now show how expectation values of observables can be computed within the general CQD ansatz of Eq. (1), while the time-evolution algorithm and parameter optimization will be discussed in the next section. As any observable can be decomposed into a sum of Pauli strings $P \in \{\mathbb{I}, X, Y, Z\}^{\otimes n}$, it suffices to consider a single arbitrary Pauli string P , the expectation value of which yields

$$\langle \psi_{\theta} | P | \psi_{\theta} \rangle = \sum_{z, z'} \psi^q(t, z)^* \psi_{\theta}^c(z)^* \psi^q(t, z') \psi_{\theta}^c(z') \langle z | P | z' \rangle. \quad (2)$$

For diagonal Pauli strings $P |z\rangle = S(z) |z\rangle$, this can be immediately written as

$$\begin{aligned} \langle \psi_{\theta} | P | \psi_{\theta} \rangle &= \sum_z |\langle z | \psi^q \rangle|^2 S(z) |\psi_{\theta}^c(z)|^2 \\ &= \mathbb{E}_{z \sim |\langle z | \psi^q \rangle|^2} [S(z) |\psi_{\theta}^c(z)|^2] \\ &\approx \frac{1}{N_s} \sum_{z \sim |\langle z | \psi^q \rangle|^2} S(z) |\psi_{\theta}^c(z)|^2, \end{aligned} \quad (3)$$

where we have dropped the time dependence for readability. The expectation value can hence be estimated by evaluating $S(z) |\psi_{\theta}^c(z)|^2$ classically at N_s configurations z sampled from the quantum circuit $|\psi^q\rangle$.

For nondiagonal observables, Zhang *et al.* [68] have shown how a more intricate measurement scheme can be exploited to similarly sample bit strings z from a quantum circuit and evaluate the classical correction accordingly. In Appendix A, we discuss the sampling procedure in detail. We show that for any Pauli string P and classical function

f , expressions of the form

$$\sum_{z, z'} \psi^q(t, z)^* \psi^q(t, z') \langle z | P | z' \rangle f(t, z, z') \quad (4)$$

can be computed by sampling configurations z from $|\psi^q\rangle$ in at most two bases. Evaluating the expectation value of a Pauli string for the CQD ansatz given in Eq. (2) is a special case of this result, with $f(t, z, z') = (\psi_{\theta(t)}^c(z))^* \psi_{\theta(t)}^c(z')$ in Eq. (4).

B. Derivation of the equations of motion

Our goal is to optimize the CQD ansatz at incremental time steps such that the resulting hybrid wave function follows the desired time evolution according to a Hamiltonian H . For an infinitesimal time step δt , we define

$$\psi_{\theta(t+\delta t)}(t + \delta t, z) = \psi_{\theta(t)+\delta\theta}^c(z) \langle z | e^{-i\delta t H} | \psi^q(t) \rangle, \quad (5)$$

where $\delta\theta$ is the update to the classical parameters that is to be determined. To that end, we apply McLachlan's variational principle [40,41],

$$\delta\theta^* = \arg \min_{\delta\theta} \| e^{-i\delta t H} | \psi_{\theta}(t) \rangle - | \psi_{\theta+\delta\theta}(t + \delta t) \rangle \|^2. \quad (6)$$

The main steps to solve this minimization problem are outlined below, assuming that the ansatz is normalized ($\langle \psi | \psi \rangle = 1$). The results are later generalized to the case of unnormalized wave functions.

Using the shorthand notation $\partial_k = \partial/\partial\theta_k$, we note that the derivative with respect to time can be expanded as

$$\frac{d}{dt} = \partial_t + \sum_k \frac{d\theta_k}{dt} \partial_k = \partial_t + \sum_k \dot{\theta}_k \partial_k. \quad (7)$$

Next, we Taylor expand both the time-evolution unitary

$$e^{-i\delta t H} = \mathbb{I} - i\delta t H + O(\delta t^2) \quad (8)$$

and the ansatz

$$| \psi_{\theta+\delta\theta}(t + \delta t) \rangle = \left(1 + \delta t \frac{d}{dt} \right) | \psi_{\theta}(t) \rangle + O(\delta t^2). \quad (9)$$

Inserting these expressions into Eq. (6) and using $\delta\theta_k = \dot{\theta}_k \delta t$, we obtain

$$\begin{aligned}
\dot{\theta}^* &= \arg \min_{\dot{\theta}} \left\| (\mathbb{1} - i\delta t H) |\psi\rangle - \left(1 + \delta t \partial_t + \delta t \sum_k \dot{\theta}_k \partial_k \right) |\psi\rangle \right\|^2 \\
&= \arg \min_{\dot{\theta}} \left\| iH |\psi\rangle + \sum_k \dot{\theta}_k |\partial_k \psi\rangle + |\partial_t \psi\rangle \right\|^2 \\
&= \arg \min_{\dot{\theta}} \sum_k \dot{\theta}_k \left[i \langle \partial_k \psi | H | \psi \rangle + \langle \partial_k \psi | \partial_t \psi \rangle + \sum_l \dot{\theta}_l (\langle \partial_k \psi | \partial_l \psi \rangle + \text{c.c.}) \right], \tag{10}
\end{aligned}$$

where we use the shorthand $|\psi\rangle = |\psi_\theta(t)\rangle$ and all terms not depending on $\dot{\theta}$ have been dropped, as they do not contribute to the arg min.

To perform the minimization, we set the derivative of the objective function with respect to $\dot{\theta}$ to zero and obtain the equations of motion for the parameter changes $\dot{\theta}$:

$$\sum_l \dot{\theta}_l \text{Re}\{\langle \partial_k \psi | \partial_l \psi \rangle\} = \text{Im}\{\langle \partial_k \psi | H | \psi \rangle\} - \text{Re}\{\langle \partial_k \psi | \partial_t \psi \rangle\}. \tag{11}$$

The generalized equations of motion for an unnormalized ansatz are given by (for the derivation, see Appendix C)

$$\sum_l S_{kl} \dot{\theta}_l = C_k - T_k, \tag{12}$$

where

$$S_{kl} = \text{Re} \left\{ \frac{\langle \partial_k \psi | \partial_l \psi \rangle}{\langle \psi | \psi \rangle} - \frac{\langle \partial_k \psi | \psi \rangle \langle \psi | \partial_l \psi \rangle}{\langle \psi | \psi \rangle^2} \right\} \tag{13}$$

is the quantum geometric tensor (QGT),

$$C_k = \text{Im} \left\{ \frac{\langle \partial_k \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} - \frac{\langle \partial_k \psi | \psi \rangle \langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle^2} \right\} \tag{14}$$

are the forces usually appearing in the equations of TDVP [40], and

$$T_k = \text{Re} \left\{ \frac{\langle \partial_k \psi | \partial_t \psi \rangle}{\langle \psi | \psi \rangle} - \frac{\langle \partial_k \psi | \psi \rangle \langle \psi | \partial_t \psi \rangle}{\langle \psi | \psi \rangle^2} \right\} \tag{15}$$

are additional forces arising from the explicit time dependence of the ansatz.

The equations of motion given in Eq. (12) can be solved using any numerical ODE integrator, such as the Euler method, to compute the parameter updates $\theta(t + \delta t)$. The TDVP time-step size δt and the choice of integrator are hyperparameters of the optimization and must be selected to balance computational cost and simulation stability.

C. Calculating the forces and the quantum geometric tensor

In Appendix B, we show that all quantities appearing in the equations of motion Eqs. (13)–(15) can be written in the form of Eq. (4). Each term can thus be computed by sampling configurations from quantum circuits (potentially in different bases) and evaluating classical functions on said samples.

As an example, the term containing the explicit time derivative appearing in the forces T_k is calculated as

$$\begin{aligned}
\langle \psi | \partial_t \psi \rangle &= \sum_z \psi^q(t, z)^* (\partial_t \psi^q(t, z)) \psi_\theta^c(z)^* \psi_\theta^c(z) \\
&= \sum_z \psi^q(t, z)^* \langle z | (-i\tilde{H}) | \psi^q(t) \rangle |\psi_\theta^c(z)|^2 \\
&= -i \sum_{z, z'} \psi^q(t, z)^* \langle z | \tilde{H} | z' \rangle \psi^q(t, z') |\psi_\theta^c(z)|^2 \\
&= -i \sum_k w_k \sum_{z, z'} \psi^q(t, z)^* \psi^q(t, z') \langle z | P_k | z' \rangle |\psi_\theta^c(z)|^2, \tag{16}
\end{aligned}$$

where we have decomposed $\tilde{H} = \sum_k w_k P_k$. This fits into the form of Eq. (4) with $f(t, z, z') = |\psi_\theta^c(z)|^2$. The corresponding results for all other terms appearing in the expressions of the QGT and forces are summarized in Table I.

At every time step, the circuit $|\psi^q(t)\rangle$ has to be sampled in a number of bases,

$$N_{\text{bases}} = 2N_{\text{nd}}(H + \tilde{H}) + 1, \tag{17}$$

where $N_{\text{nd}}(H + \tilde{H})$ are the numbers of nondiagonal Pauli strings in the Pauli decomposition of H and $\tilde{H}$, respectively. The factor of 2 appears as different bases have to be chosen to obtain the real and imaginary parts of the expectation values. Note that if Pauli strings are contained in both Hamiltonians, the samples can be reused and, hence, $N_{\text{nd}}(H + \tilde{H}) \leq N_{\text{nd}}(H) + N_{\text{nd}}(\tilde{H})$.

TABLE I. All the quantities appearing in the equations of motion can be recast to expressions of the form given in Eq. (4). Here, we list the Pauli strings according to which the time-evolved circuit has to be sampled and the classical functions that have to be evaluated on those samples to compute each expression. We write $\mathcal{P}(H)$ to denote the set of Pauli strings appearing in the decomposition of H .

Expression	Pauli strings	$f(t, z, z')$
$\langle \psi \psi \rangle$	Identity	$ \psi_\theta^c(z) ^2$
$\langle \partial_t \psi \partial_k \psi \rangle$	Identity	$(\partial_t \psi_\theta^c(z))^* \partial_k \psi_\theta^c(z)$
$\langle \partial_k \psi \psi \rangle$	Identity	$(\partial_k \psi_\theta^c(z))^* \psi_\theta^c(z)$
$\langle \psi H \psi \rangle$	$P \in \mathcal{P}(H)$	$(\psi_\theta^c(z))^* \psi_\theta^c(z')$
$\langle \partial_k \psi H \psi \rangle$	$P \in \mathcal{P}(H)$	$(\partial_k \psi_\theta^c(z))^* \psi_\theta^c(z')$
$\langle \psi \partial_t \psi \rangle$	$P \in \mathcal{P}(\tilde{H})$	$ \psi_\theta^c(z) ^2$
$\langle \partial_k \psi \partial_t \psi \rangle$	$P \in \mathcal{P}(\tilde{H})$	$(\partial_k \psi_\theta^c(z))^* \psi_\theta^c(z)$

III. APPLICATIONS

In this section, we present three use cases that illustrate how the CQD ansatz can be leveraged to correct or extend Trotterized quantum dynamics. First, we demonstrate its ability to mitigate Trotter errors. Second, we show how the CQD framework enables hardware-efficient time evolution on a quantum computer, even for Hamiltonians with nonlocal terms. Finally, we explore how additional degrees of freedom can be incorporated entirely within the classical component of the ansatz, eliminating the need for extra qubits on the quantum device. Note that these examples are not exhaustive but highlight the versatility and potential of the CQD ansatz for quantum dynamics simulations.

A. Correcting Trotter errors

In order to implement the time-evolution unitary $U(t) = \exp(-iHt)$ for general Hamiltonians as a quantum circuit, we usually employ a Trotterization of $U(t)$. For a Hamiltonian with noncommuting terms $[H_k, H_l] \neq 0$, we can expand to, e.g., first order

$$\exp(-iHt) = \left(\prod_k \exp(-iH_k \Delta t) \right)^{t/\Delta t} + O(t\Delta t), \quad (18)$$

which is a good approximation for small Trotter steps Δt . The benefit of this Trotterization is that individual terms can now be efficiently implemented as a quantum circuit through a product of locally acting quantum gates. In practice, on noisy devices we only have access to a limited number of Trotter steps due to the restricted coherence time. This leads to a trade-off between Trotter error and hardware noise.

Here, we demonstrate how our hybrid method can be used to address this problem. To this end, we can interpret Trotterized time evolution as exact quantum evolution with an effective piecewise constant Hamiltonian (see Fig. 2).

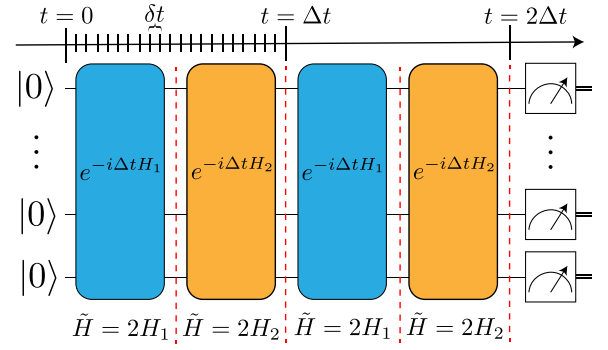


FIG. 2. A quantum circuit representing two first-order Trotter steps of a Hamiltonian $H = H_1 + H_2$, where H_1 and H_2 are two noncommuting terms. To correct for the error arising from the large Trotter steps Δt , we update the classical ansatz at a smaller timescale δt . Within this timescale, the unitary $e^{-i\Delta t H_i}$ can be seen as a time evolution according to an effective Hamiltonian $\tilde{H} = 2H_i$ for a time $\Delta t/2$. Note that we show a first-order Trotter step here to simplify the visualization. In practice, we employ second-order Trotterization in our experiments to obtain a higher-order approximation at the cost of a constant-depth unitary transformation.

For example, the first-order Trotter decomposition for a Hamiltonian $H = H_1 + H_2$ is written as

$$\begin{aligned} |\psi(t + \Delta t)\rangle &= \exp(-iH\Delta t) |\psi(t)\rangle \\ &\approx \exp(-iH_2\Delta t) \exp(-iH_1\Delta t) |\psi(t)\rangle \\ &= \exp\left(-2iH_2\frac{\Delta t}{2}\right) \exp\left(-2iH_1\frac{\Delta t}{2}\right) |\psi(t)\rangle. \end{aligned} \quad (19)$$

A Trotter step can thus be described within our framework by setting $\tilde{H} = 2H_1$ for the first half of the time step Δt and $\tilde{H} = 2H_2$ during the second half. This generalizes for multiple Trotter steps, Hamiltonians with more than two terms, and higher-order Trotter decompositions. Given an expressive enough classical ansatz ψ_θ^c and a TDVP timescale $\delta t \ll \Delta t$, we can thus correct errors arising from coarse Trotterization.

As an example, we simulate the transverse-field Ising model (TFIM) on a chain of $L = 10$ spins with open boundary conditions, described by the Hamiltonian

$$H = -h \sum_{i=1}^L X_i - J \sum_{i=1}^L Z_i Z_{i+1}, \quad (20)$$

where we set the local field $h = 1$ and the coupling strength $J = 2$. X_i and Z_i denote the corresponding Pauli operators acting on the i th qubit. We start in the $+1$ eigenstate of the X basis $|\psi_0\rangle = |+\rangle^{\otimes L}$ and evolve it in time using Trotterization to second order with a Trotter step size $\Delta t = 0.25$. The TDVP time step is set to $\delta t = 0.005$ and we integrate

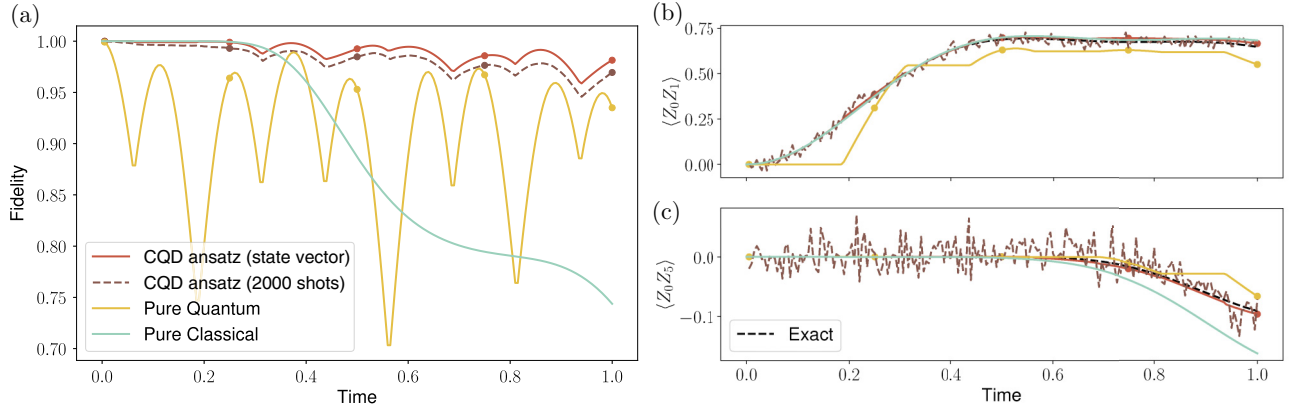


FIG. 3. Correcting Trotter errors in the simulation of the TFIM on a chain of ten spins with open boundary conditions. (a) The fidelity of the simulated quantum states with respect to the exact solution. We compare a purely classical simulation based on a Jastrow ansatz (blue line) as defined in Eq. (21) with the CQD ansatz combining the Jastrow with the Trotterized quantum circuit for both a noiseless (red line) and a shot-based simulation (dashed brown line). The uncorrected quantum simulation is displayed for reference (yellow line). (b),(c) The ZZ correlation (b) between the first two qubits and (c) between an edge and a central qubit. The exact expectation values are shown in black. The Trotterization is chosen at second order with time-step size $\Delta t = 0.25$ (full Trotter steps are indicated with dots).

the equations of motion using the Euler method. Note that here we can in fact split the Hamiltonian into two noncommuting terms, $H = H_x + H_z$, where H_x contains the local fields whereas H_z consists of the couplings.

As the classical model, we choose a simple Jastrow ansatz [71] given by

$$\psi_\theta^c(z) = \exp \left(\sum_i \theta_i z_i + \sum_{ij} \theta_{ij} z_i z_j \right), \quad (21)$$

where all parameters are complex and the two-body parameters are symmetric: $\theta_{ij} = \theta_{ji}$. For L spins, we count a total of $L + [L(L-1)/2]$ complex parameters. The parameters are initialized to $\theta(0) = 0$, such that $\psi_{\theta(0)}^c(z) \equiv 1$.

In Fig. 3(a), we plot and compare the fidelities of quantum states simulated by different means with respect to the exact solution

$$F(|\psi_\theta(t)\rangle, |\psi_{\text{exact}}\rangle) = |\langle \psi_\theta(t) | e^{-iHt} | \psi_0 \rangle|^2. \quad (22)$$

Simulating the evolution using solely the Trotterized quantum circuit approximation without the classical model (yellow line) gives rise to oscillating nonsmooth fidelities. Cusps appear whenever the piecewise constant evolution is switched between H_x and H_z . The points in time at which a full Trotter step is completed are marked with dots. In contrast, simulating the system purely with a classical Jastrow ansatz without the help of the quantum circuit (blue line) results in a smooth fidelity curve, which, however, quickly drops for times $t \gtrsim 0.3$. Hence, the Jastrow ansatz alone is not expressive enough to capture the dynamics of the system at large times.

Finally, we combine the Trotterized circuit and the Jastrow ansatz within our CQD framework. We show both an ideal state-vector simulation (solid red line) and a shot-based simulation (dashed brown line) with 2000 shots per evaluated circuit [72]. In each case, we obtain fidelities superior to the purely quantum and purely classical simulation for $t \gtrsim 0.3$. Hence, the CQD ansatz allows for an accurate simulation using a classical ansatz with fewer parameters that would otherwise not be sufficient to capture the full dynamics of the system alone (this point is further investigated in Appendix D). Furthermore, the nonsmooth oscillating behavior stemming from the Trotterization is washed out, also resulting in high fidelities of the simulated CQD state at intermediate times in between Trotter steps.

To obtain a better understanding of the expressibility of the ansatz, we additionally plot two observables. In Fig. 5(b), we show the correlator $\langle Z_0 Z_1 \rangle$ of two neighboring spins. For this local observable, the Jastrow ansatz alone is able to capture the dynamics faithfully for the entire evolution. However, when we examine the correlator $\langle Z_0 Z_5 \rangle$ between an edge and a central spin, we observe that only the CQD ansatz provides an accurate prediction over the entire time window [see Fig. 5(c)]. This indicates that the quantum circuit is required for the simulation of long-range correlations, whereas the Jastrow ansatz is needed to correct the arising Trotter error and interpolate the dynamics between the discrete Trotter steps. The latter is apparent for both observables; the Trotterized evolution without the classical correction gives rise to piecewise constant expectation values whenever the state is evolved according to the Hamiltonian H_z (as this Hamiltonian commutes with the observable). However, even at times

that match a full Trotter step (yellow dots), the simulated expectation values are less accurate than those predicted by the CQD ansatz due to the Trotter error. Note that the statistical noise apparent in the shot-based simulation could be alleviated by increasing the number of shots.

B. Hardware-efficient time evolution

Qubit connectivity in near-term quantum hardware, such as for superconducting qubits, is often restricted by the topology given by the device. For example, IBM Quantum hardware follows a heavy-hex topology [73] and Google's Willow processor is connected in a square lattice [74]. Applying two-qubit gates between qubits that are not connected with native hardware connections requires additional SWAP gates, which greatly increases the circuit depth and thus the required coherence time to successfully run the circuit. This problem arises when, e.g., evolving a quantum state in time with respect to a Hamiltonian that does not follow the hardware topology. Here, we propose to evolve the quantum state with a hardware-efficient approximation of the Hamiltonian. We only include those terms of H that respect the topology of the device in $\tilde{H}$, where $\tilde{H}$ again denotes the effective Hamiltonian that governs the dynamics on the quantum computer. We then use a classical ansatz to correct for the nonlocal terms in H that have been omitted in the approximation $\tilde{H}$.

As an example, we consider a two-dimensional TFIM with nearest-neighbor coupling J_1 and next-nearest-neighbor coupling J_2 in a grid of 3×3 spins (see Fig. 4)

$$\begin{aligned} H &= -h \sum_i X_i - J_1 \sum_{\langle ij \rangle} Z_i Z_j - J_2 \sum_{\langle\langle ij \rangle\rangle} Z_i Z_j \\ &= \tilde{H} - J_2 \sum_{\langle\langle ij \rangle\rangle} Z_i Z_j. \end{aligned} \quad (23)$$

We assume that the nearest-neighbor interaction is much stronger, $J_1 \gg J_2$, such that the part of the Hamiltonian that only includes the local field and nearest-neighbor couplings, $\tilde{H}$, is a good approximation of the total Hamiltonian H . In this case, we can employ a simple classical model (such as a Jastrow ansatz [71]) to correct the total dynamics with the hybrid CQD scheme. In Fig. 4, we show how the exclusion of nonlocal terms (yellow lines and gates) reduces the circuit depth significantly even given an all-to-all qubit connectivity. For a quantum device with nearest-neighbor interactions, the benefit would be even greater as SWAP gates would be required to implement all the next-nearest-neighbor interacting terms not included in $\tilde{H}$.

The initial state is chosen as $|\psi_0\rangle = |+\rangle^{\otimes 9}$ and the classical parameters are initialized at zero. To implement the dynamics as a quantum circuit, the time evolution is Trotterized to second order with $\Delta t = 0.1$, where the CQD

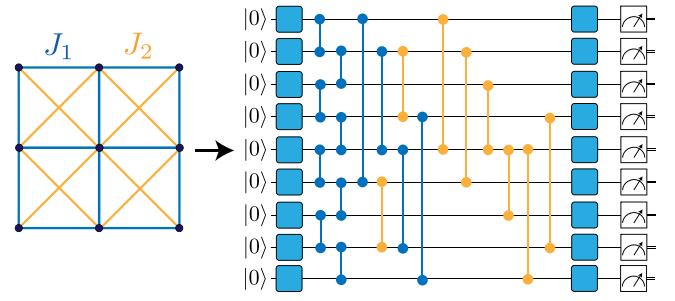


FIG. 4. The two-dimensional spin system with strong nearest-neighbor (J_1) and weak next-nearest-neighbor interaction (J_2). The left panel shows the topology of the system, where the nodes indicate individual spins with a local field h and the edges represent the couplings $J_{ij} Z_i \otimes Z_j$. The right panel shows the circuit implementing a single second-order Trotter step for such a system, with boxes representing the R_X rotations and lines between qubits the R_{ZZ} gates. Even without including the required SWAP gates, the circuit depth can be significantly reduced when omitting the next-nearest-neighbor couplings (yellow lines and gates).

ansatz is additionally tasked with correcting the Trotter error as described in Sec. III A. We use the Euler method with $\delta t = 0.005$ to integrate the equations of motion.

In Fig. 5, we show the fidelities and two correlated observables of the simulation with the CQD ansatz compared to a purely quantum simulation (ignoring next-nearest-neighbor terms) and a purely classical version. The hardware-efficient circuit alone (yellow line) is not able to capture the full dynamics. This is to be expected given that the next-nearest-neighbor terms are completely neglected in that case. Additionally, the effect of the Trotterization is apparent through an oscillating fidelity and piecewise continuous expectation values of the correlated observables $\langle Z_1 Z_9 \rangle$ [Fig. 5(b)] and $\langle X_1 X_9 \rangle$ [Fig. 5(c)]. On the other hand, the Jastrow ansatz optimized purely classically (blue line) performs better but also fails to provide a faithful simulation for longer times due to its limited expressivity.

Finally, the CQD ansatz combining the quantum circuit with the Jastrow ansatz achieves the highest fidelity. We plot the state-vector simulation (red line) and compare it to shot-based simulations (brown lines) with different numbers of shots per evaluated circuit. Note that while in these cases the ansatz is optimized with shot noise, the fidelity is always computed using the full state. As expected, the quality of the simulation improves as the number of shots increases. However, already for a modest number of 1000 shots, we observe an improvement in fidelity at later times over the classical Jastrow ansatz and the hardware-efficient circuit alone. These results suggest that we are indeed able to correct the quantum circuit evolution for missing terms in the Hamiltonian and, consequently, reduce the circuit depth as well as avoid SWAP gates.

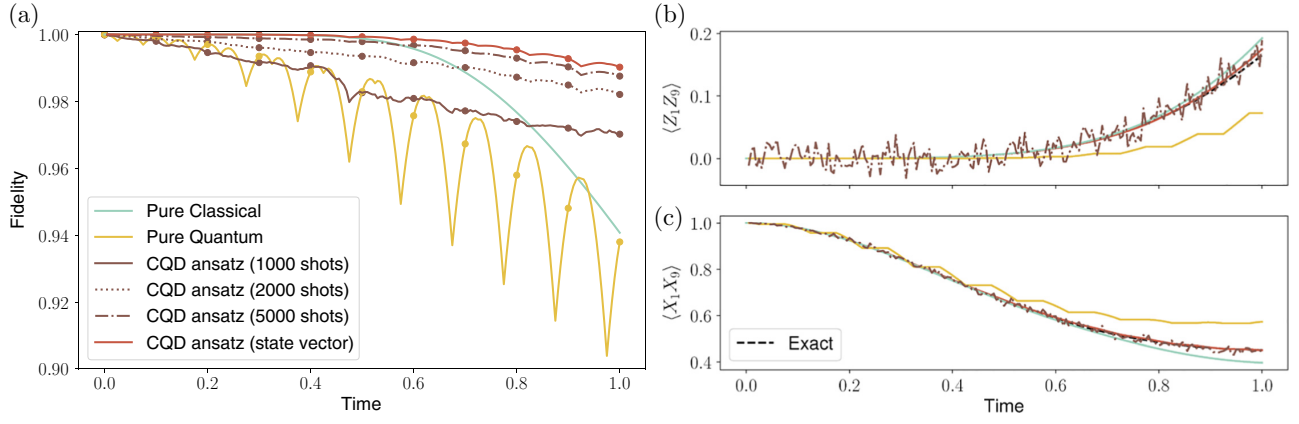


FIG. 5. Reducing the circuit depth by simulating the TFIM setup displayed in Fig. 4 with the CQD ansatz, where the quantum circuit only includes nearest-neighbor couplings and the classical correction is chosen as a Jastrow ansatz. The Hamiltonian parameters are $J_1 = 0.5$, $J_2 = 0.1$, and $h = 1$. The Trotter decomposition is chosen at second order with $\Delta t = 0.1$. (a) The fidelity of the quantum simulation neglecting next-nearest-neighbor terms (yellow line), of the purely classical simulation (blue line), and of the CQD ansatz for different numbers of shots (red and brown lines). (b),(c) The (b) ZZ and (c) XX correlation between the top-left and bottom-right spins in Fig. 4. For visibility, we only include the simulation with 5000 shots.

C. Extending the system size

In this section, we discuss how the hybrid ansatz can be employed to expand the system size by including additional degrees of freedom in the classical model. This is particularly useful if the system can be split into two subsystems, where one subsystem is highly correlated and benefits from the simulation on a quantum computer, whereas the second subsystem is only weakly correlated and can be simulated classically. The extended CQD ansatz takes as input configurations of both the highly correlated part z_q and the weakly correlated bath z_c and is defined as

$$\begin{aligned} \psi_{\theta(t+\delta t)}(t + \delta t, z_c, z_q) &= \psi_{\theta(t)+\delta\theta}^c(z_c, z_q) \langle z_q | e^{-i\delta t \tilde{H}} | \psi^q(t) \rangle \\ &= \psi_{\theta(t)+\delta\theta}^c(z_c, z_q) \psi^q(t + \delta t, z_q), \end{aligned} \quad (24)$$

where $\tilde{H}$ is a Hamiltonian that only acts on the highly correlated subsystem simulated on the quantum device. For a general Hamiltonian of the form $H = H_q + H_c + H_{qc}$, where H_c (H_q) acts on the classically treated bath (quantum) degrees of freedom and H_{qc} acts on both systems, a straightforward choice is $\tilde{H} = H_q$.

When computing expectation values of observables with the extended CQD ansatz, we can no longer sample the full configurations over the whole system on the quantum device. Instead, we sample only z_q from the quantum circuit and use alternative classical ways of sampling the bath configurations z_c . To this end, we redefine the classical contribution of the wave function as

$$\psi_{\theta}^c(z_c, z_q) = \psi_{\theta}^{c_1}(z_q) \psi_{\theta}^{c_2}(z_q, z_c), \quad (25)$$

where the factor depending on z_c is constrained to be normalized according to

$$\sum_{z_c} |\psi_{\theta}^{c_2}(z_c, z_q)|^2 = 1, \quad \forall z_q. \quad (26)$$

Using this ansatz, z_c can be directly sampled from $|\psi_{\theta}^{c_2}(z_c, z_q)|^2$ given z_q . Further, to calculate the total normalization appearing in Eqs. (13)–(15), no sampling of the classical configuration z_c is required, since

$$\begin{aligned} \langle \psi_{\theta} | \psi_{\theta} \rangle &= \sum_{z_q, z_c} |\psi_{\theta}(z_q, z_c)|^2 \\ &= \sum_{z_q} |\psi^q(z_q)|^2 |\psi_{\theta}^{c_1}(z_q)|^2 \sum_{z_c} |\psi_{\theta}^{c_2}(z_c, z_q)|^2 \\ &= \sum_{z_q} |\psi^q(z_q)|^2 |\psi_{\theta}^{c_1}(z_q)|^2. \end{aligned} \quad (27)$$

In Appendix B 1, we show how these properties allow us to compute all the quantities in the TDVP equations of motion in a similar fashion, as discussed in Sec. II C.

To test the extended CQD ansatz, we simulate a TFIM on a line partitioned into two subsystems (see Fig. 6). Four central spins, referred to as the *quantum partition*, are connected with nearest-neighbor coupling strength $J_q = 1$. Both ends of the chain are further connected to a bath chain of $n_c/2$ spins with an interaction strength $J_{qc} = 0.25$. The bath spins themselves are connected with a nearest-neighbor coupling of $J_c = 0.1$ and can thus be regarded as only weakly correlated. The local fields are set to $h = 1$ over the whole system. On the quantum device, we evolve the central spins according to $\tilde{H}$, which contains the terms

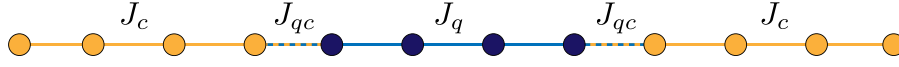


FIG. 6. A spin chain in a TFIM split into four strongly correlated spins in the middle (blue), which are treated on a quantum device. The remaining (bath) spins (yellow) are weakly correlated and treated purely classically.

of H that only act on this partition (excluding the coupling between quantum and bath subsystems).

We choose the same Jastrow ansatz, given in Eq. (21), as in the previous sections for the classical ansatz $\psi_{\theta}^{c1}(z_q)$ acting only on the strongly correlated spins. The bath chains are represented by a mean-field ansatz ψ_{θ}^{c2} , defined as

$$\psi_{\theta}^{c2}(z_q, z_c) = \prod_{i=1}^{n_c} \frac{e^{\lambda_{\theta}(z_q)_i z_c^{(i)}}}{\sqrt{e^{2\text{Re}\{\lambda_{\theta}(z_q)_i\}} + e^{-2\text{Re}\{\lambda_{\theta}(z_q)_i\}}}}, \quad (28)$$

where λ_{θ} is a function parametrized by θ and taking a quantum configuration z_q as input. As a consequence, the parameters of the mean-field ansatz are no longer fixed but depend on the configurations sampled from the quantum circuit z_q through the function λ_{θ} . This dependence serves as a backaction between the two subsystems and is essential to allow for correlations between them. Indeed, in our framework, the classical ansatz is the only way in which the bath can influence the dynamics of the spins simulated on the quantum device, as this evolution is kept unitary and performed independently of the bath.

We choose a neural network with one hidden layer with $2n_c$ neurons and a tanh activation function to map $z_q \mapsto \lambda_{\theta}(z_q)$. During the time evolution, we hence have to

update both the parameters in the Jastrow ansatz ψ_{θ}^{c1} and the weights and biases of this neural network.

The mean-field ansatz allows for exact sampling of z_c given z_q by sampling each spin individually from the normalized distribution

$$p_i(z_c^{(i)}) = \frac{e^{2\text{Re}\{\lambda_{\theta}(z_q)_i z_c^{(i)}\}}}{e^{2\text{Re}\{\lambda_{\theta}(z_q)_i\}} + e^{-2\text{Re}\{\lambda_{\theta}(z_q)_i\}}}. \quad (29)$$

The initial state is once again chosen as $|\psi_0\rangle = |+\rangle^{\otimes(n_q+n_c)}$. We set the parameters of ψ_{θ}^{c1} as well as the weights and biases of the final layer of the neural network to zero to ensure that $\psi_{\theta(0)}^c(z_c, z_q) \equiv 1$ at time $t = 0$. The remaining parameters are initialized randomly to avoid vanishing forces. We use second-order Trotterization with $\Delta t = 0.1$ and integrate the equations of motion using the Euler method with $\delta t = 0.001$.

In Fig. 7(a), we plot the fidelity of the CQD simulation with respect to the exact solution for different numbers of bath spins n_c (red and brown lines). In addition, we include the fidelity obtained by optimizing the same classical ansatz $\psi_{\theta}^c(z_c, z_q)$ without the help of a quantum circuit using TDVP provided by the NetKet PYTHON library [75] (blue lines). The purely classical simulation achieves high fidelities up to $t \lesssim 0.5$, when the fidelity starts to significantly drop for all considered system sizes. In contrast, for

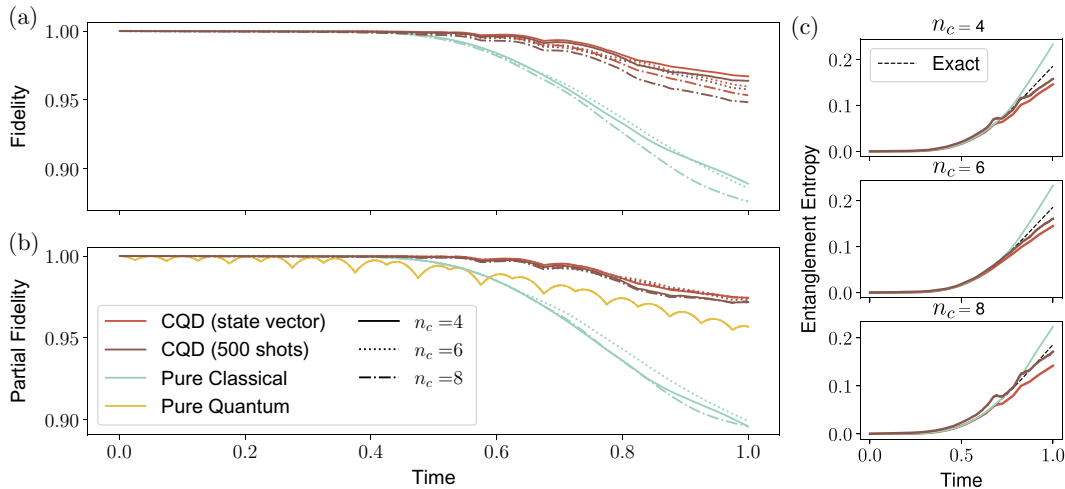


FIG. 7. Extending the system size by simulating the TFIM on two subsystems as portrayed in Fig. 6 using a Jastrow ansatz on the quantum partition and a mean-field ansatz for the classical spins. We compare how the CQD ansatz (state vector in red and shot-based in brown) performs compared to a purely classical (in cyan) simulation with the same classical ansatz for different numbers of bath spins n_c . (a) The global fidelity compared to the exact solution. (b) The fidelity of the reduced states, where the bath spins have been traced out. Here, we also include the fidelity of the Trotterized quantum circuit without the classical correction (yellow line). (c) A plot of the entanglement entropy between the two subsystems, compared to the exact solution (in black).

the CQD ansatz, the fidelity stays high for the whole evolution. These results again demonstrate that incorporating the quantum circuit into a simple classical ansatz increases its expressivity, allowing for more accurate simulations at longer times.

In addition to the state-vector simulation, we perform a shot-based simulation with the CQD ansatz (brown lines). To that end, we sample 500 configurations z_q from every circuit. Given z_q , we then sample ten classical configurations z_c from the mean-field ansatz. In Fig. 7, we show that the shot-based optimization is able to reach a comparable fidelity to the state-vector results, indicating that a modest number of shots (and, similarly, a small number of classical samples) is sufficient for the system sizes considered here.

Note that we observe a slight decrease in the accuracy of the simulation for increasing bath sizes n_c —which, however, is to be expected, as the classical bath partition is modeled using a mean-field ansatz and thus the many-body fidelity naturally decreases with the bath size. Hence, to further study the system-size dependency and simulation accuracy on the quantum partition alone, we compute the partial fidelity of the evolved quantum state [see Fig. 7(b)], where we trace out the bath spins

$$F_q(\rho, \sigma) = \text{Tr} \left[\sqrt{\sqrt{\rho_q} \sigma_q \sqrt{\rho_q}} \right]^2, \quad (30)$$

where $\rho_q = \text{Tr}_c[\rho] = \text{Tr}_c[|\psi\rangle\langle\psi|]$ is the reduced state. The partial fidelity of the purely classical simulation drops after $t \sim 0.5$, similar to the global fidelity. The purely quantum evolution that ignores the bath spins (yellow line) shows the usual oscillatory behavior due to the Trotterization with a partial fidelity that slowly decreases on average but already obtains superior results compared to the classical simulation. Finally, the CQD ansatz yields the highest partial fidelities throughout the time evolution. In contrast to the global fidelity, the partial fidelity reached by CQD remains unaffected by the number of bath spins included in the simulation, both for the state-vector and shot-based simulations. Moreover, the improved accuracy of the hybrid CQD ansatz compared to the purely quantum evolution demonstrates that the classical ansatz allows for information to propagate back from the bath into the quantum partition and thus is able to capture correlations between the subsystems.

To further study this correlation, in Fig. 7(c), we plot the von Neumann entanglement entropy between the quantum and classical partition defined on the reduced density matrix ρ_q [76]

$$E[\rho_q] = -\text{Tr} [\rho_q \log(\rho_q)]. \quad (31)$$

We find that the backaction between the bath and quantum partitions introduced with the neural network indeed

allows us to recover the entanglement between the two subsystems, independent of the size of the bath.

Overall, these results demonstrate that the CQD ansatz enables an extension of the system size through a simple classical ansatz, which alone would lack the expressiveness required for accurately simulating the dynamics over longer timescales. We expect this to be the case whenever a part of the system can be efficiently simulated classically. If both partitions behave highly nonclassically or if the entanglement between the two partitions is too large, a quantum device might be required for the full system to obtain faithful simulations. In that case, the CQD method could still be employed to correct for Trotter errors or simplify the Hamiltonian by omitting long-range gates, as discussed in the previous subsections.

IV. DISCUSSION AND OUTLOOK

In this work, we introduce a method that leverages classical simulation techniques to correct and extend Trotterized dynamics of quantum many-body systems on near-term quantum hardware. By exploiting the strengths of quantum computers, such as their ability to capture growing entanglement during time evolution, while relying on classical methods to mitigate their limitations, such as restricted connectivity and limited coherence time, we provide a new near-term quantum-classical algorithm for the simulation of quantum dynamics.

The key principle of our method is that the quantum circuit is evolved with respect to an approximation of the full Hamiltonian. This approximation is then corrected by iteratively updating the parameters of a classical ansatz using TDVP. To obtain the correct equations of motion, we extend TDVP to the case in which the ansatz contains an explicit time dependence. Crucially, the subroutine run on the quantum computer only consists of Trotterized time evolution and sampling configurations in easily preparable bases. Since the quantum circuit has no variational parameters, the forces and the quantum geometric tensor required for TDVP can be evaluated purely classically, given samples from the quantum device. This eliminates the need for computationally demanding tasks such as calculating complex overlaps (e.g., using the Hadamard test) or gradients (e.g., using the parameter-shift rule) on a quantum computer.

We demonstrate that incorporating a simple Jastrow ansatz in a coarsely Trotterized dynamics simulation of the TFIM significantly improves the quantum state fidelity. This shows that our CQD framework can be employed to correct Trotter errors often arising in digital quantum simulations with near-term hardware. Furthermore, we show that the ansatz allows for the simulation of long-range Hamiltonians while keeping the quantum circuit hardware efficient. To that end, we simulate a two-dimensional TFIM with strong nearest-neighbor and

weaker next-nearest-neighbor coupling strengths. Finally, the CQD ansatz allows to increase the system size beyond the available qubits of the quantum device. We demonstrate this by using a classical mean-field ansatz to incorporate additional spins that are treated purely classically. Each of these applications highlights the capability of the hybrid CQD ansatz in enhancing the accuracy of approximate dynamics simulation on quantum hardware.

Moreover, we show that the CQD ansatz leverages the approximate simulation on the quantum device to increase the expressivity compared to a purely classical ansatz. This enables the use of simpler classical ansatz with fewer parameters to simulate highly entangled systems, where such ansatz would otherwise fail. Reducing the number of variational parameters is particularly beneficial, as the inversion of the quantum geometric tensor is prone to instabilities when employing complex ansatz with a large number of parameters [77].

In this paper, we touch upon three applications of the method. However, these are by no means exhaustive. On the contrary, the proposed ansatz opens the door to any system in which the time evolution can only be implemented approximately on the quantum device. As long as the effective Hamiltonian acting on the quantum partition is known, our framework can be used to correct the dynamics with a sufficiently expressive classical ansatz. Furthermore, the ability of the CQD ansatz to extend system sizes—provided that the additional degrees of freedom are efficiently classically simulable—suggests its applicability to a variety of physically interesting systems. Examples include molecular systems that can be partitioned into active and inactive orbitals [78,79] or quantum impurity models [80,81]. Finally, note that our derivation of TDVP with an explicit time dependence is general and can be employed in any dynamics simulation—classical or quantum—and with any parametrized ansatz that contains an explicit time dependence.

There are numerous potential extensions and improvements to the CQD ansatz. The framework itself is kept deliberately general, particularly with regard to the choice of classical ansatz. While we primarily discuss the Jastrow ansatz, alternative classical wave functions—such as tensor networks [82] or neural-network quantum states [83]—could also be considered. Additionally, a scaling analysis using near-term quantum hardware would be valuable in assessing the performance of the method under realistic noise conditions.

We would also like to note that our method presents a framework to correct quantum dynamics in postprocessing. In contrast, prior works [84–86] have aimed to reduce Trotter errors by optimizing the quantum circuit implementing the time-evolution unitary. This can be achieved by minimizing a loss function based on a perturbative expansion of the Trotter error [84] or by preoptimizing circuits using tensor-network approaches [85,86]. While

we focus on Trotterized time evolution in this paper, the method is in principle agnostic to how the unitary $U = \exp(-it\tilde{H})$ is implemented on the quantum device. Therefore, the CQD method could be combined with arbitrary preprocessing methods to further reduce the depth of U .

The fact that the time evolution does not necessarily have to be implemented using Trotterization also implies that the method could still be of relevance in an early fault-tolerant era. In particular, the application presented in Sec. III C remains important. As the number of logical qubits will still be limited in the coming decades, it remains crucial to only employ quantum resources where they are necessarily required. If part of a system can be treated effectively classically, our method allows for the efficient simulation of such a system using reduced quantum resources. In this case, the time-evolution unitary could also be implemented using fault-tolerant techniques such as qubitization [87].

Currently, the main bottleneck of the CQD framework is the fact that quantum circuits have to be sampled frequently, as the TDVP time step has to be chosen small enough to allow for a stable and accurate numerical integration of the equations of motion. We note that this is a problem that arises similarly in variational quantum time-evolution algorithms, where the circuit not only needs to be sampled at each time step, but complex overlaps have to be computed [29–32,41] or loss functions have to be optimized [33–36]. Therefore, our algorithm comes at a smaller cost in terms of quantum resources compared to other near-term quantum time-evolution algorithms. Nevertheless, exploring alternative ways of sampling the quantum circuits is an interesting direction for future research.

While we do not present results from current NISQ hardware in this work, our method is designed with near-term devices in mind and we expect it to be implementable within existing experimental constraints. While our scheme does not explicitly incorporate error mitigation, the hybrid architecture offers a potential form of implicit error mitigation. By allowing a classical model to correct errors introduced by coarse Trotterization or simplified dynamics, we can limit quantum evolution to shallow circuits, possibly just a few Trotter steps. In this regime, Trotter error, rather than hardware noise, could become the dominant source of inaccuracy, which is then directly corrected by the classical model.

ACKNOWLEDGMENTS

We thank Stefano Barison, Jannes Nys, Linda Mauron, and Alessandro Sinibaldi for insightful discussions on hybrid methods and the time-dependent variational principle for classical ansatz, as well as Shao-Hen Chiew and Samuele Piccinelli for valuable feedback on the

manuscript. This research was supported by the NCCR MARVEL, a National Centre of Competence in Research, funded by the Swiss National Science Foundation (Grant No. 205602).

DATA AVAILABILITY

The data that support the findings of this paper are openly available [88].

CODE AVAILABILITY

The code to run the CQD ansatz is available as a PYTHON package on GitHub [88]. The repository contains the simulations performed in this paper as examples and provides a general framework to simulate the dynamics of arbitrary Hamiltonians where the classical ansatz can easily be interchanged. It is built upon JAX [89], FLAX [90], NetKet [75] and PENNYLANE [91].

APPENDIX A: MEASURING NONDIAGONAL OBSERVABLES AND FORCES

In Sec. II, we show how all the quantities required for the time evolution with the CQD ansatz as well as the measurement of observables can be written in the form

$$E(P, f) = \sum_{z, z'} \psi^q(t, z)^* \psi^q(t, z') \langle z | P | z' \rangle f(t, z, z'). \quad (\text{A1})$$

For diagonal Pauli strings, recasting this sum as a sampling problem is straightforward (see the discussion in Sec. II A). For off-diagonal Pauli strings, we employ the strategy proposed by Zhang *et al.* [68]. First note that a Pauli string P maps every computational basis state z to another computational basis state $\tilde{z}$ up to a phase $S(\tilde{z}) \in \{\pm 1, \pm i\}$. We thus write $Pz = S(\tilde{z})\tilde{z}$, which allows us to eliminate the sum over z' as

$$\begin{aligned} E(P, f) &= \sum_{z, z'} \psi^q(z)^* \psi^q(z') \langle \tilde{z} | S(z) | z' \rangle f(z, z') \\ &= \sum_z \psi^q(z)^* \psi^q(\tilde{z}) S(z) f(z, \tilde{z}) \\ &= \sum_z \langle \psi^q | z \rangle \langle \tilde{z} | \psi^q \rangle S(z) f(z, \tilde{z}) \end{aligned}$$

$$= \langle \psi^q | \left[\sum_z S(z) f(z, \tilde{z}) | z \rangle \langle \tilde{z} | \right] | \psi^q \rangle, \quad (\text{A2})$$

where we have dropped the time dependence for readability and used $S(\tilde{z})^* = S(z)$. We now reorder the qubits such that the Pauli acting on the first qubit P_0 is nondiagonal, i.e., either X or Y . As such, if $z_0 = 0$ we have $\tilde{z}_0 = 1$ and vice versa, which allows us to rewrite the sum by fixing $z_0 = 0$ as

$$\begin{aligned} E(P, f) &= \langle \psi^q | \left[\sum_{z, \text{s.t. } z_0=0} S(z) f(z, \tilde{z}) | z \rangle \langle \tilde{z} | \right. \\ &\quad \left. + S(\tilde{z}) f(\tilde{z}, z) | \tilde{z} \rangle \langle z | \right] | \psi^q \rangle. \quad (\text{A3}) \end{aligned}$$

Each term in this sum can be written as

$$\begin{aligned} &f(z, \tilde{z}) S(z) | z \rangle \langle \tilde{z} | + f(\tilde{z}, z) S(\tilde{z}) | \tilde{z} \rangle \langle z | \\ &= \frac{1}{2} (f(z, \tilde{z}) + f(\tilde{z}, z)) (S(z) | z \rangle \langle \tilde{z} | + S(\tilde{z}) | \tilde{z} \rangle \langle z |) \\ &\quad + \frac{1}{2} (f(z, \tilde{z}) - f(\tilde{z}, z)) (S(z) | z \rangle \langle \tilde{z} | - S(\tilde{z}) | \tilde{z} \rangle \langle z |) \\ &= \frac{1}{2} (f(z, \tilde{z}) + f(\tilde{z}, z)) \\ &\quad (|+, z_{1:n-1}\rangle \langle +, z_{1:n-1}| - |- , z_{1:n-1}\rangle \langle - , z_{1:n-1}|) \\ &\quad + \frac{i}{2} (f(z, \tilde{z}) - f(\tilde{z}, z)) \\ &\quad (|+i, z_{1:n-1}\rangle \langle +i, z_{1:n-1}| - |-i, z_{1:n-1}\rangle \langle -i, z_{1:n-1}|), \quad (\text{A4}) \end{aligned}$$

where

$$\begin{aligned} |\pm, z_{1:n-1}\rangle &= \frac{1}{\sqrt{2}} (S(z) |0, z_{1:n-1}\rangle \pm |1, \tilde{z}_{1:n-1}\rangle), \\ |\pm i, z_{1:n-1}\rangle &= \frac{1}{\sqrt{2}} (S(z) |0, z_{1:n-1}\rangle \pm i |1, \tilde{z}_{1:n-1}\rangle). \quad (\text{A5}) \end{aligned}$$

Note that these states can easily be prepared using controlled Pauli operations. In the case in which $P_0 = X$ and hence $S(z_0) = 1$, we find

$$\begin{aligned} |+, z_{1:n-1}\rangle &= (|0\rangle \langle 0| \otimes \mathbb{I}_{n-1} + |1\rangle \langle 1| \otimes P_{1:n-1}) (H \otimes \mathbb{I}_{n-1}) (|0\rangle \otimes |z_{1:n-1}\rangle), \\ |- , z_{1:n-1}\rangle &= (|0\rangle \langle 0| \otimes \mathbb{I}_{n-1} + |1\rangle \langle 1| \otimes P_{1:n-1}) (H \otimes \mathbb{I}_{n-1}) (|1\rangle \otimes |z_{1:n-1}\rangle), \\ |+i, z_{1:n-1}\rangle &= (|0\rangle \langle 0| \otimes \mathbb{I}_{n-1} + |1\rangle \langle 1| \otimes P_{1:n-1}) (SH \otimes \mathbb{I}_{n-1}) (|0\rangle \otimes |z_{1:n-1}\rangle), \\ |-i, z_{1:n-1}\rangle &= (|0\rangle \langle 0| \otimes \mathbb{I}_{n-1} + |1\rangle \langle 1| \otimes P_{1:n-1}) (SH \otimes \mathbb{I}_{n-1}) (|1\rangle \otimes |z_{1:n-1}\rangle), \quad (\text{A6}) \end{aligned}$$

where H is the Hadamard and S is the phase gate. For $P_0 = Y$ with $S(z_0) = i$, we need an extra $-S$ gate, resulting in

$$\begin{aligned} |+, z_{1:n-1}\rangle &= (|0\rangle\langle 0| \otimes \mathbb{I}_{n-1} + |1\rangle\langle 1| \otimes P_{1:n-1}) ((-S)H \otimes \mathbb{I}_{n-1}) (|0\rangle \otimes |z_{1:n-1}\rangle), \\ |-, z_{1:n-1}\rangle &= (|0\rangle\langle 0| \otimes \mathbb{I}_{n-1} + |1\rangle\langle 1| \otimes P_{1:n-1}) ((-S)H \otimes \mathbb{I}_{n-1}) (|1\rangle \otimes |z_{1:n-1}\rangle), \\ |+i, z_{1:n-1}\rangle &= (|0\rangle\langle 0| \otimes \mathbb{I}_{n-1} + |1\rangle\langle 1| \otimes P_{1:n-1}) (H \otimes \mathbb{I}_{n-1}) (|0\rangle \otimes |z_{1:n-1}\rangle), \\ |-i, z_{1:n-1}\rangle &= (|0\rangle\langle 0| \otimes \mathbb{I}_{n-1} + |1\rangle\langle 1| \otimes P_{1:n-1}) (H \otimes \mathbb{I}_{n-1}) (|1\rangle \otimes |z_{1:n-1}\rangle). \end{aligned} \quad (\text{A7})$$

In summary, we are able to rewrite

$$\begin{aligned} E(P, f) &= \frac{1}{2} \sum_{z_{1:n-1}} |\langle \psi^q | +, z_{1:n-1} \rangle|^2 (f(z, \tilde{z}) + f(\tilde{z}, z)) \\ &\quad - \frac{1}{2} \sum_{z_{1:n-1}} |\langle \psi^q | -, z_{1:n-1} \rangle|^2 (f(z, \tilde{z}) + f(\tilde{z}, z)) \\ &\quad + \frac{i}{2} \sum_{z_{1:n-1}} |\langle \psi^q | +i, z_{1:n-1} \rangle|^2 (f(z, \tilde{z}) + f(\tilde{z}, z)) \\ &\quad - \frac{i}{2} \sum_{z_{1:n-1}} |\langle \psi^q | -i, z_{1:n-1} \rangle|^2 (f(z, \tilde{z}) + f(\tilde{z}, z)), \end{aligned} \quad (\text{A8})$$

which allows us to evaluate the expectation value by sampling z from the time-evolved circuit in the basis corresponding to either Eq. (A6) or Eq. (A7) and evaluating the classical function $f(z, \tilde{z})$ accordingly on those samples.

APPENDIX B: DERIVATION OF TABLE I

In this appendix, we provide the derivations for Table I, which describes how all the terms appearing in the equations of motion Eq. (12) can be written in the form of Eq. (4).

We start with the norm

$$\langle \psi | \psi \rangle = \sum_z |\psi^q(t, z)|^2 |\psi_\theta^c(z)|^2, \quad (\text{B1})$$

which corresponds to Eq. (4) for $P = I$ and $f(t, z, z') = |\psi_\theta^c(z)|^2$. Moving on to the quantum geometric tensor, we find

$$\langle \partial_l \psi | \partial_k \psi \rangle = \sum_z |\psi^q(t, z)|^2 (\partial_l \psi_\theta^c(z))^* \partial_k \psi_\theta^c(z), \quad (\text{B2})$$

which again corresponds to the identity Pauli with $f(t, z, z') = (\partial_l \psi_\theta^c(z))^* \partial_k \psi_\theta^c(z)$. Similarly, the results for $\langle \partial_k \psi | \psi \rangle$ and $\langle \psi | \partial_k \psi \rangle$ can be found.

Moving on to the forces, we now have to decompose the Hamiltonian into Pauli strings $H = \sum_i w_i P_i$ to find

$$\begin{aligned} \langle \partial_k \psi | H | \psi \rangle &= \sum_i w_i \langle \partial_k \psi | P_i | \psi \rangle \\ &= \sum_i w_i \sum_{z, z'} \psi^q(t, z)^* \psi^q(t, z') \langle z | P_i | z' \rangle (\partial_k \psi_\theta^c(z))^* \psi_\theta^c(z'), \end{aligned} \quad (\text{B3})$$

corresponding to Eq. (4), where the circuit needs to be sampled for every Pauli string in the decomposition of H and the function to be evaluated is $f(t, z, z') = (\partial_k \psi_\theta^c(z))^* \psi_\theta^c(z')$. Similarly, the results for $\langle \psi | H | \psi \rangle$ can be found.

The derivation for $\langle \psi | \partial_t \psi \rangle$ is given in the main text and the results for $\langle \partial_k \psi | \partial_t \psi \rangle$ are found equivalently.

1. Derivation for the case of two subsystems

In this section, we provide the same calculations as above for the case in which additional degrees of freedom are added purely classically. As in the main text, we assume that the global ansatz is given as

$$\begin{aligned} \psi_{\theta(t+\delta t)}(t + \delta t, z_c, z_q) &= \psi^q(t + \delta t, z_q) \psi_{\theta(t)+\delta\theta}^c(z_c, z_q) \\ &= \psi^q(t + \delta t, z_q) \psi_{\theta(t)+\delta\theta}^{c1}(z_q) \psi_{\theta(t)+\delta\theta}^{c2}(z_c, z_q), \end{aligned} \quad (\text{B4})$$

with

$$1 = \sum_{z_c} |\psi_{\theta}^{c2}(z_c, z_q)|^2 \quad \forall z_q. \quad (\text{B5})$$

In addition to the challenge of sampling z_c described in the main text, we have to consider Pauli strings that act on either or both partitions. We write $P = P^c \otimes P^q$ for Pauli strings appearing in the decomposition of H . Note that, in contrast, $\tilde{H}$ only acts on the quantum partition. We use the notation $P|z\rangle = S(\tilde{z})|\tilde{z}\rangle$ introduced in Appendix A to denote the connected elements of a Pauli string P . We further assume that the classical functions are given in the form

$$\psi_{\theta}^{c1}(z_q) = \exp(\varphi_{\theta}^{c1}(z_q)), \quad \psi_{\theta}^{c2}(z_c, z_q) = \exp(\varphi_{\theta}^{c2}(z_c, z_q)), \quad (\text{B6})$$

such that the derivatives can be written as

$$\partial_k \psi_\theta^c(z_c, z_q) = \partial_k \exp(\varphi_\theta^{c1}(z_q) + \varphi_\theta^{c2}(z_c, z_q)) = \psi_\theta^c(z_c, z_q) \partial_k (\varphi_\theta^{c1}(z_q) + \varphi_\theta^{c2}(z_c, z_q)) = \psi_\theta^c(z_c, z_q) \partial_k \varphi_\theta^c(z_c, z_q), \quad (\text{B7})$$

where we have defined $\varphi_\theta^c(z_c, z_q) = \varphi_\theta^{c1}(z_q) + \varphi_\theta^{c2}(z_c, z_q)$.

With this notation, we can now write the force for $H = \sum_i w_i P_i$ as

$$\begin{aligned} \langle \partial_k \psi | H | \psi \rangle &= \sum_i w_i \sum_{z_q, z'_q} \psi^q(z_q)^* \psi^q(z'_q) \langle z_q | P_i^q | z'_q \rangle \sum_{z_c, z'_c} (\partial_k \psi_\theta^c(z_c, z_q))^* \psi_\theta^c(z'_c, z'_q) \langle z_c | P_i^c | z'_c \rangle \\ &= \sum_i w_i \sum_{z_q, z'_q} \psi^q(z_q)^* \psi^q(z'_q) \langle z_q | P_i^q | z'_q \rangle f_i(t, z_q, z'_q), \end{aligned} \quad (\text{B8})$$

where the classical functions to be evaluated can be written as

$$\begin{aligned} f_i(t, z_q, z'_q) &= \psi_\theta^{c1}(z_q)^* \psi_\theta^{c1}(z'_q) \sum_{z_c, z'_c} \psi_\theta^{c2}(z_c, z_q)^* \psi_\theta^{c2}(z'_c, z'_q) (\partial_k \varphi_\theta^c(z_c, z_q))^* \langle z_c | P_i^c | z'_c \rangle \\ &= \psi_\theta^{c1}(z_q)^* \psi_\theta^{c1}(z'_q) \sum_{z_c} \psi_\theta^{c2}(z_c, z_q)^* \psi_\theta^{c2}(\tilde{z}_c, z'_q) (\partial_k \varphi_\theta^c(z_c, z_q))^* S_i(z_c) \\ &= \psi_\theta^{c1}(z_q)^* \psi_\theta^{c1}(z'_q) \sum_{z_c} |\psi_\theta^{c2}(z_c, z_q)|^2 \frac{\psi_\theta^{c2}(\tilde{z}_c, z'_q)}{\psi_\theta^{c2}(z_c, z_q)} (\partial_k \varphi_\theta^c(z_c, z_q))^* S_i(z_c) \\ &= \psi_\theta^{c1}(z_q)^* \psi_\theta^{c1}(z'_q) \mathbb{E}_{z_c \sim |\psi_\theta^{c2}(z_c, z_q)|^2} \left[\frac{\psi_\theta^{c2}(\tilde{z}_c, z'_q)}{\psi_\theta^{c2}(z_c, z_q)} (\partial_k \varphi_\theta^c(z_c, z_q))^* S_i(z_c) \right]. \end{aligned} \quad (\text{B9})$$

For each sampled z_q , we thus have to estimate an expectation value by sampling z_c from $|\psi_\theta^{c2}(z_c, z_q)|^2$. The remaining terms can be found similarly and are listed in Table II.

TABLE II. All the expressions appearing in the equations of motion can be computed using the form provided in Eq. (4) for the case of two subsystems described in Sec. III C. Here, we list the Pauli strings according to which the circuit has to be sampled and the classical functions that have to be evaluated to compute each expression. We write $\mathcal{P}(H)$ to denote the set of Pauli strings appearing in the decomposition of H . We use the shorthand $z_c \sim z_q$ for z_c sampled from $|\psi_\theta^{c2}(z_c, z_q)|^2$ given z_q .

Expression	Pauli strings	$f(t, z_q, z'_q)$
$\langle \psi \psi \rangle$	Identity	$ \psi_\theta^{c1}(z_q) ^2$
$\langle \partial_t \psi \partial_k \psi \rangle$	Identity	$ \psi_\theta^{c1}(z_q) ^2 \mathbb{E}_{z_c \sim z_q} [(\partial_t \varphi_\theta^c(z_c, z_q))^* \partial_k \varphi_\theta^c(z_c, z_q)]$
$\langle \partial_k \psi \psi \rangle$	Identity	$ \psi_\theta^{c1}(z_q) ^2 \mathbb{E}_{z_c \sim z_q} [(\partial_k \varphi_\theta^c(z_c, z_q))^*]$
$\langle \psi H \psi \rangle$	$P_i^c \otimes P_i^q \in \mathcal{P}(H)$	$\psi_\theta^{c1}(z_q)^* \psi_\theta^{c1}(z'_q) \mathbb{E}_{z_c \sim z_q} \left[\frac{\psi_\theta^{c2}(\tilde{z}_c, z'_q)}{\psi_\theta^{c2}(z_c, z_q)} S_i(z_c) \right]$
$\langle \partial_k \psi H \psi \rangle$	$P_i^c \otimes P_i^q \in \mathcal{P}(H)$	$\psi_\theta^{c1}(z_q)^* \psi_\theta^{c1}(z'_q) \mathbb{E}_{z_c \sim z_q} \left[\frac{\psi_\theta^{c2}(\tilde{z}_c, z'_q)}{\psi_\theta^{c2}(z_c, z_q)} (\partial_k \varphi_\theta^c(z_c, z_q))^* S_i(z_c) \right]$
$\langle \psi \partial_t \psi \rangle$	$P_i^q \in \mathcal{P}(\tilde{H})$	$ \psi_\theta^{c1}(z_q) ^2$
$\langle \partial_k \psi \partial_t \psi \rangle$	$P_i^q \in \mathcal{P}(\tilde{H})$	$ \psi_\theta^{c1}(z_q) ^2 \mathbb{E}_{z_c \sim z_q} [(\partial_k \varphi_\theta^c(z_c, z_q))^*]$

APPENDIX C: TDVP FOR UNNORMALIZED WAVE FUNCTIONS

The derivation of the TDVP equations in the main text assumes that the ansatz remains normalized over time. To generalize this to unnormalized classical wave functions and to address the problem of the global phase being ignored in McLachlan's principle, we add two additional virtual parameters to the ansatz, which will modify the equations of motion. We add the parameter θ_0^R to encode the normalization and θ_0^I to fix the global phase. The total ansatz now takes the form

$$\psi_{\theta(t)}(t, z) = e^{\theta_0^R(t) + i\theta_0^I(t)} \psi_{\theta(t)}^c(z) \psi^q(t, z), \quad (C1)$$

where the classical ansatz $\psi_{\theta(t)}^c$ still only depends on the original parameters θ . To derive the new equations of

motion for $\theta_{k>1}$, we first observe that

$$|\partial_{\theta_0^R} \psi\rangle = \sum_z \partial_{\theta_0^R} \psi_{\theta(t)}(t, z) |z\rangle = \sum_z \psi_{\theta(t)}(t, z) |z\rangle = |\psi\rangle \quad (C2)$$

and, similarly,

$$|\partial_{\theta_0^I} \psi\rangle = i|\psi\rangle. \quad (C3)$$

The equations of motion in Eq. (11) for the virtual parameters $k = 0$ are thus given by

$$\begin{aligned} \dot{\theta}_0^R \langle \psi | \psi \rangle + \sum_{l>0} \dot{\theta}_l \text{Re}\{\langle \partial_l \psi | \psi \rangle\} &= -\text{Re}\{\langle \psi | \partial_l \psi \rangle\} \\ \dot{\theta}_0^I \langle \psi | \psi \rangle - \sum_{l>0} \dot{\theta}_l \text{Im}\{\langle \partial_l \psi | \psi \rangle\} &= -\langle \psi | H | \psi \rangle - \text{Im}\{\langle \psi | \partial_l \psi \rangle\}. \end{aligned} \quad (C4)$$

We can now plug these results into the equation of motions for $k > 0$ to obtain, for the left-hand side,

$$\begin{aligned} \sum_l \dot{\theta}_l \text{Re}\{\langle \partial_l \psi | \partial_k \psi \rangle\} &= \dot{\theta}_0^R \text{Re}\{\langle \psi | \partial_k \psi \rangle\} + \dot{\theta}_0^I \text{Im}\{\langle \psi | \partial_k \psi \rangle\} + \sum_{l>0} \dot{\theta}_l \text{Re}\{\langle \partial_l \psi | \partial_k \psi \rangle\} \\ &= -\sum_{l>0} \dot{\theta}_l \frac{\text{Re}\{\langle \partial_l \psi | \psi \rangle\} \text{Re}\{\langle \psi | \partial_k \psi \rangle\}}{\langle \psi | \psi \rangle} - \frac{\text{Re}\{\langle \psi | \partial_l \psi \rangle\} \text{Re}\{\langle \psi | \partial_k \psi \rangle\}}{\langle \psi | \psi \rangle} \\ &\quad + \sum_{l>0} \dot{\theta}_l \frac{\text{Im}\{\langle \partial_l \psi | \psi \rangle\} \text{Im}\{\langle \psi | \partial_k \psi \rangle\}}{\langle \psi | \psi \rangle} - \frac{\langle \psi | H | \psi \rangle \text{Im}\{\langle \psi | \partial_k \psi \rangle\}}{\langle \psi | \psi \rangle} \\ &\quad - \frac{\text{Im}\{\langle \psi | \partial_l \psi \rangle\} \text{Im}\{\langle \psi | \partial_k \psi \rangle\}}{\langle \psi | \psi \rangle} + \sum_{l>0} \dot{\theta}_l \text{Re}\{\langle \partial_l \psi | \partial_k \psi \rangle\} \\ &= \sum_{l>0} \dot{\theta}_l \left(\text{Re}\{\langle \partial_l \psi | \partial_k \psi \rangle\} - \frac{\text{Re}\{\langle \partial_l \psi | \psi \rangle\} \text{Re}\{\langle \psi | \partial_k \psi \rangle\}}{\langle \psi | \psi \rangle} \right) \\ &\quad - \frac{\text{Re}\{\langle \partial_k \psi | \psi \rangle\} \text{Re}\{\langle \psi | \partial_l \psi \rangle\}}{\langle \psi | \psi \rangle} + \frac{\text{Im}\{\langle \partial_k \psi | \psi \rangle\} \text{Im}\{\langle \psi | H | \psi \rangle\}}{\langle \psi | \psi \rangle}. \end{aligned} \quad (C5)$$

Setting this equal to the right-hand side of Eq. (11), dividing both sides by $\langle \psi | \psi \rangle$, and rearranging yields the equations of motion for an unnormalized ansatz,

$$\sum_{l>0} S_{kl} \dot{\theta}_l = C_k - T_k, \quad (C6)$$

where

$$S_{kl} = \text{Re} \left\{ \frac{\langle \partial_l \psi | \partial_k \psi \rangle}{\langle \psi | \psi \rangle} - \frac{\langle \partial_l \psi | \psi \rangle \langle \psi | \partial_k \psi \rangle}{\langle \psi | \psi \rangle^2} \right\} \quad (C7)$$

is the geometric tensor,

$$C_k = \text{Im} \left\{ \frac{\langle \partial_k \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} - \frac{\langle \partial_k \psi | \psi \rangle \langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle^2} \right\} \quad (C8)$$

are the usual forces, and

$$T_k = \text{Re} \left\{ \frac{\langle \partial_k \psi | \partial_l \psi \rangle}{\langle \psi | \psi \rangle} - \frac{\langle \partial_k \psi | \psi \rangle \langle \psi | \partial_l \psi \rangle}{\langle \psi | \psi \rangle^2} \right\} \quad (C9)$$

are additional forces arising from the explicit time dependence of the ansatz.

APPENDIX D: SIMPLIFYING CLASSICAL OPTIMIZATION BY ENHANCING QUANTUM SIMULATION ACCURACY

In this appendix, we provide an additional experiment to showcase how the accuracy of the simulation increases as the Hamiltonian acting on the quantum device $\tilde{H}$ approaches the target Hamiltonian H . The Hamiltonian setup is the same as in Sec. III A, where we choose the quantum time evolution to be exact, i.e., without any Trotter error. Instead, we fix the approximation of the Hamiltonian on the quantum device to be proportional to the true Hamiltonian through $\tilde{H} = \alpha H$. In particular, the simulation is purely classical for $\alpha = 0$ and purely quantum for $\alpha = 1$.

In Fig. 8, we vary α from 0.75 to 1 and plot the fidelity as a function of time. We use the same Jastrow ansatz given by Eq. (21) throughout all experiments. Additionally, we compare the simulations to the edge case $\alpha = 0$ (dashed black line). It is apparent that the fidelity of the simulation improves as $\tilde{H}$ approaches H .

This experiment demonstrates how increasing the accuracy of the quantum simulation simplifies the classical optimization task. For $\alpha \ll 1$, the Jastrow ansatz is not expressive enough to capture the full dynamics. As α increases, this manifests in the forces T_k appearing in the equations of motion given in Eq. (12), which are directly proportional to α [see Eq. (16)]. These heuristics support the intuition that including the forces T_k arising from a good approximation $\tilde{H}$ of H makes the problem posed by the equations of motion easier to solve. This allows for simple classical ansatz with a small number of parameters to effectively capture the dynamics.

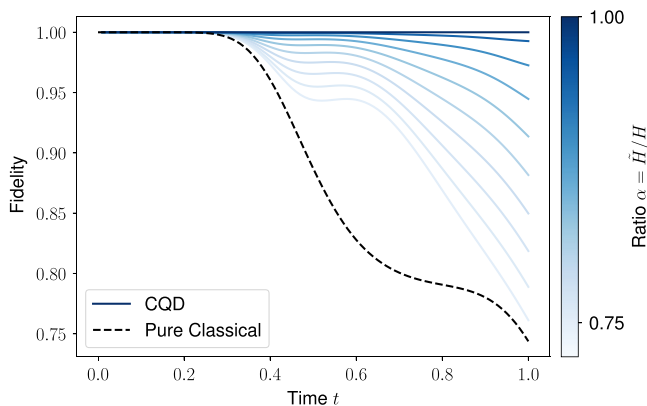


FIG. 8. The time evolution of the transverse-field Ising model for $J = 2$, $h = 1$ using the CQD ansatz, in which the Hamiltonian acting on the quantum device is varied as $\tilde{H} = \alpha H$. From the purely classical case $\alpha = 0$, the fidelity of the simulation gradually improves as α approaches 1.

- [1] J. Zhang, G. Pagano, P. W. Hess, A. Kyprianidis, P. Becker, H. Kaplan, A. V. Gorshkov, Z. X. Gong, and C. Monroe, Observation of a many-body dynamical phase transition with a 53-qubit quantum simulator, *Nature* **551**, 601 (2017).
- [2] J. Dborin, V. Wimalaweera, F. Barratt, E. Ostby, T. E. O'Brien, and A. G. Green, Simulating groundstate and dynamical quantum phase transitions on a superconducting quantum computer, *Nat. Commun.* **13**, 5977 (2022).
- [3] 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).
- [4] E. Altman, Many-body localization and quantum thermalization, *Nat. Phys.* **14**, 979 (2018).
- [5] W. A. de Jong, K. Lee, J. Mulligan, M. Płoskoń, F. Ringer, and X. Yao, Quantum simulation of nonequilibrium dynamics and thermalization in the Schwinger model, *Phys. Rev. D* **106**, 054508 (2022).
- [6] Y. Kim, A. Eddins, S. Anand, K. X. Wei, E. van den Berg, S. Rosenblatt, H. Nayfeh, Y. Wu, M. Zaletel, K. Temme, and A. Kandala, Evidence for the utility of quantum computing before fault tolerance, *Nature* **618**, 500 (2023).
- [7] G. Vidal, Efficient classical simulation of slightly entangled quantum computations, *Phys. Rev. Lett.* **91**, 147902 (2003).
- [8] J. Eisert, M. Friesdorf, and C. Gogolin, Quantum many-body systems out of equilibrium, *Nat. Phys.* **11**, 124 (2015).
- [9] D. Bauernfeind and M. Aichhorn, Time dependent variational principle for tree tensor networks, *SciPost Phys.* **8**, 024 (2020).
- [10] A. Sinibaldi, C. Giuliani, G. Carleo, and F. Vicentini, Unbiasing time-dependent variational Monte Carlo by projected quantum evolution, *Quantum* **7**, 1131 (2023).
- [11] J. Nys, Z. Denis, and G. Carleo, Real-time quantum dynamics of thermal states with neural thermofields, *Phys. Rev. B* **109**, 235120 (2024).
- [12] L. Mauron, Z. Denis, J. Nys, and G. Carleo, Predicting topological entanglement entropy in a Rydberg analogue simulator, *Nat. Phys.* **21**, 1332 (2025).
- [13] A. Sinibaldi, D. Hendry, F. Vicentini, and G. Carleo, Time-dependent neural Galerkin method for quantum dynamics, *ArXiv:2412.11778*.
- [14] L. Mauron and G. Carleo, Challenging the quantum advantage frontier with large-scale classical simulations of annealing dynamics, *ArXiv:2503.08247*.
- [15] R. P. Feynman, Simulating physics with computers, *Int. J. Theor. Phys.* **21**, 467 (1982).
- [16] A. Kandala, A. Mezzacapo, K. Temme, M. Takita, M. Brink, J. M. Chow, and J. M. Gambetta, Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets, *Nature* **549**, 242 (2017).
- [17] A. Chiesa, F. Tacchino, M. Grossi, P. Santini, I. Tavernelli, D. Gerace, and S. Carretta, Quantum hardware simulating four-dimensional inelastic neutron scattering, *Nat. Phys.* **15**, 455 (2019).
- [18] F. Arute, *et al.*, Hartree-Fock on a superconducting qubit quantum computer, *Science* **369**, 1084 (2020).
- [19] F. Arute, *et al.*, Observation of separated dynamics of charge and spin in the Fermi-Hubbard model, *ArXiv:2010.07965*.

- [20] C. Neill, *et al.*, Accurately computing the electronic properties of a quantum ring, *Nature* **594**, 508 (2021).
- [21] J. Preskill, Quantum computing in the NISQ era and beyond, *Quantum* **2**, 79 (2018).
- [22] A. M. Childs, D. Maslov, Y. Nam, N. J. Ross, and Y. Su, Toward the first quantum simulation with quantum speedup, *Proc. Natl. Acad. Sci.* **115**, 9456 (2018).
- [23] R. Babbush, C. Gidney, D. W. Berry, N. Wiebe, J. McClean, A. Paler, A. Fowler, and H. Neven, Encoding electronic spectra in quantum circuits with linear T complexity, *Phys. Rev. X* **8**, 041015 (2018).
- [24] Y. Nam and D. Maslov, Low-cost quantum circuits for classically intractable instances of the Hamiltonian dynamics simulation problem, *npj Quantum Inf.* **5**, 44 (2019).
- [25] M. Motta, E. Ye, J. R. McClean, Z. Li, A. J. Minnich, R. Babbush, and G. K.-L. Chan, Low rank representations for quantum simulation of electronic structure, *npj Quantum Inf.* **7**, 83 (2021).
- [26] N. Hatano and M. Suzuki, in *Quantum Annealing and Other Optimization Methods* (Springer-Verlag, Berlin, 2005), p. 37.
- [27] D. W. Berry, G. Ahokas, R. Cleve, and B. C. Sanders, Efficient quantum algorithms for simulating sparse Hamiltonians, *Commun. Math. Phys.* **270**, 359 (2006).
- [28] K. Bharti, A. Cervera-Lierta, T. H. Kyaw, T. Haug, S. Alperin-Lea, A. Anand, M. Degroote, H. Heimonen, J. S. Kottmann, T. Menke, W.-K. Mok, S. Sim, L.-C. Kwek, and A. Aspuru-Guzik, Noisy intermediate-scale quantum algorithms, *Rev. Mod. Phys.* **94**, 015004 (2022).
- [29] X. Yuan, S. Endo, Q. Zhao, Y. Li, and S. C. Benjamin, Theory of variational quantum simulation, *Quantum* **3**, 191 (2019).
- [30] M. Benedetti, M. Fiorentini, and M. Lubasch, Hardware-efficient variational quantum algorithms for time evolution, *Phys. Rev. Res.* **3**, 033083 (2021).
- [31] F. Zhang, C.-Z. Wang, T. Iadecola, P. P. Orth, and Y.-X. Yao, Adaptive variational quantum dynamics simulations with compressed circuits and fewer measurements, *Phys. Rev. B* **111**, 094310 (2025).
- [32] J. Gacon, C. Zoufal, G. Carleo, and S. Woerner, Simultaneous perturbation stochastic approximation of the quantum Fisher information, *Quantum* **5**, 567 (2021).
- [33] S. Barison, F. Vicentini, and G. Carleo, An efficient quantum algorithm for the time evolution of parameterized circuits, *Quantum* **5**, 512 (2021).
- [34] D. Linteau, S. Barison, N. H. Lindner, and G. Carleo, Adaptive projected variational quantum dynamics, *Phys. Rev. Res.* **6**, 023130 (2024).
- [35] G. Gentinetta, F. Metz, and G. Carleo, Overhead-constrained circuit knitting for variational quantum dynamics, *Quantum* **8**, 1296 (2024).
- [36] 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).
- [37] J. S. Gacon, Ph.D. thesis, École polytechnique fédérale de Lausanne (EPFL), 2024, <https://doi.org/10.5075/EPFL-THESIS-11132>.
- [38] P. A. M. Dirac, Note on exchange phenomena in the Thomas atom, *Math. Proc. Camb. Philos. Soc.* **26**, 376 (1930).
- [39] J. Frenkel, *Wave Mechanics: Advanced General Theory* (Oxford University Press, London, 1934).
- [40] A. McLachlan, A variational solution of the time-dependent Schrödinger equation, *Mol. Phys.* **8**, 39 (1964).
- [41] Y. Li and S. C. Benjamin, Efficient variational quantum simulator incorporating active error minimization, *Phys. Rev. X* **7**, 021050 (2017).
- [42] K. Mitarai, M. Negoro, M. Kitagawa, and K. Fujii, Quantum circuit learning, *Phys. Rev. A* **98**, 32309 (2018).
- [43] M. Schuld, V. Bergholm, C. Gogolin, J. Izaac, and N. Kilorian, Evaluating analytic gradients on quantum hardware, *Phys. Rev. A* **99**, 032331 (2019).
- [44] A. Abbas, R. King, H.-Y. Huang, W. J. Huggins, R. Movassagh, D. Gilboa, and J. McClean, On quantum backpropagation, information reuse, and cheating measurement collapse, in *Advances in Neural Information Processing Systems*, edited by A. Oh, T. Naumann, A. Globerson, K. Saenko, M. Hardt, and S. Levine (Curran Associates, Inc., 2023), Vol. 36, pp. 44792–44819, https://proceedings.neurips.cc/paper_files/paper/2023/file/8c3caae2f725c8e2a55ecd600563d172-Paper-Conference.pdf.
- [45] C. Cirstoiu, Z. Holmes, J. Iosue, L. Cincio, P. J. Coles, and A. Sornborger, Variational fast forwarding for quantum simulation beyond the coherence time, *npj Quantum Inf.* **6**, 82 (2020).
- [46] B. Commeau, M. Cerezo, Z. Holmes, L. Cincio, P. J. Coles, and A. Sornborger, Variational Hamiltonian diagonalization for dynamical quantum simulation, *ArXiv:2009.02559*.
- [47] C. L. Cortes, A. E. DePrince, and S. K. Gray, Fast-forwarding quantum simulation with real-time quantum Krylov subspace algorithms, *Phys. Rev. A* **106**, 042409 (2022).
- [48] K. Heya, K. M. Nakanishi, K. Mitarai, Z. Yan, K. Zuo, Y. Suzuki, T. Sugiyama, S. Tamate, Y. Tabuchi, K. Fujii, and Y. Nakamura, Subspace variational quantum simulator, *Phys. Rev. Res.* **5**, 023078 (2023).
- [49] H. Zhao, M. Bukov, M. Heyl, and R. Moessner, Making Trotterization adaptive and energy-self-correcting for NISQ devices and beyond, *PRX Quantum* **4**, 030319 (2023).
- [50] H. Zhao, M. Bukov, M. Heyl, and R. Moessner, Adaptive Trotterization for time-dependent Hamiltonian quantum dynamics using piecewise conservation laws, *Phys. Rev. Lett.* **133**, 010603 (2024).
- [51] S. Bravyi, G. Smith, and J. A. Smolin, Trading classical and quantum computational resources, *Phys. Rev. X* **6**, 021043 (2016).
- [52] T. Peng, A. W. Harrow, M. Ozols, and X. Wu, Simulating large quantum circuits on a small quantum computer, *Phys. Rev. Lett.* **125**, 150504 (2020).
- [53] K. Mitarai and K. Fujii, Constructing a virtual two-qubit gate by sampling single-qubit operations, *New J. Phys.* **23**, 023021 (2021).
- [54] K. Mitarai and K. Fujii, Overhead for simulating a non-local channel with local channels by quasiprobability sampling, *Quantum* **5**, 388 (2021).
- [55] C. Piveteau and D. Sutter, Circuit knitting with classical communication, *IEEE Trans. Inf. Theory* **70**, 2734 (2023).

- [56] Z. Fan and Q.-L. Jie, Cluster density matrix embedding theory for quantum spin systems, *Phys. Rev. B* **91**, 195118 (2015).
- [57] K. Gunst, S. Wouters, S. De Baerdemacker, and D. Van Neck, Block product density matrix embedding theory for strongly correlated spin systems, *Phys. Rev. B* **95**, 195127 (2017).
- [58] T. Yamazaki, S. Matsuura, A. Narimani, A. Saidmuradov, and A. Zaribafiyani, Towards the practical application of near-term quantum computers in quantum chemistry simulations: A problem decomposition approach, *ArXiv:1806.01305*.
- [59] M. Rossmannek, P. K. Barkoutsos, P. J. Ollitrault, and I. Tavernelli, Quantum HF/DFT-embedding algorithms for electronic structure calculations: Scaling up to complex molecular systems, *J. Chem. Phys.* **154**, 114105 (2021).
- [60] A. Eddins, M. Motta, T. P. Gujarati, S. Bravyi, A. Mezzacapo, C. Hadfield, and S. Sheldon, Doubling the size of quantum simulators by entanglement forging, *PRX Quantum* **3**, 010309 (2022).
- [61] P. Huembeli, G. Carleo, and A. Mezzacapo, Entanglement forging with generative neural network models, *ArXiv:2205.00933*.
- [62] P. de Schouepnikoff, O. Kiss, S. Vallecorsa, G. Carleo, and M. Grossi, Hybrid ground-state quantum algorithms based on neural Schrödinger forging, *Phys. Rev. Res.* **6**, 023021 (2024).
- [63] S. Barison, F. Vicentini, and G. Carleo, Embedding classical variational methods in quantum circuits, *ArXiv:2309.08666*.
- [64] X. Yuan, J. Sun, J. Liu, Q. Zhao, and Y. Zhou, Quantum simulation with hybrid tensor networks, *Phys. Rev. Lett.* **127**, 040501 (2021).
- [65] J. Sun, S. Endo, H. Lin, P. Hayden, V. Vedral, and X. Yuan, Perturbative quantum simulation, *Phys. Rev. Lett.* **129**, 120505 (2022).
- [66] J. Schuhmacher, M. Ballarin, A. Baiardi, G. Magnifico, F. Tacchino, S. Montangero, and I. Tavernelli, Hybrid tree tensor networks for quantum simulation, *PRX Quantum* **6**, 010320 (2025).
- [67] A. McClain Gomez, T. L. Patti, A. Anandkumar, and S. F. Yelin, Near-term distributed quantum computation using mean-field corrections and auxiliary qubits, *Quantum Sci. Technol.* **9**, 035022 (2024).
- [68] S.-X. Zhang, Z.-Q. Wan, C.-K. Lee, C.-Y. Hsieh, S. Zhang, and H. Yao, Variational quantum-neural hybrid eigensolver, *Phys. Rev. Lett.* **128**, 120502 (2022).
- [69] W. Dobrutz, I. O. Sokolov, K. Liao, P. L. Ríos, M. Rahm, A. Alavi, and I. Tavernelli, Toward real chemical accuracy on current quantum hardware through the transcorrelated method, *J. Chem. Theory Comput.* **20**, 4146 (2024).
- [70] F. Metz, G. Pescia, and G. Carleo, Simulating continuous-space systems with quantum-classical wave functions, *ArXiv:2409.06415*.
- [71] R. Jastrow, Many-body problem with strong forces, *Phys. Rev.* **98**, 1479 (1955).
- [72] The simulation is performed using shot noise. However, to compute the fidelities, we use the full state vectors.
- [73] J. Gambetta, Expanding the IBM quantum roadmap to anticipate the future of quantum-centric supercomputing (2022), <https://research.ibm.com/blog/ibm-quantum-roadmap-2025>.
- [74] R. Acharya, *et al.*, Quantum error correction below the surface code threshold, *Nature* **638**, 920 (2024).
- [75] F. Vicentini, D. Hofmann, A. Szabó, D. Wu, C. Roth, C. Giuliani, G. Pescia, J. Nys, V. Vargas-Calderón, N. Astrakhantsev, and G. Carleo, NetKet 3: Machine learning toolbox for many-body quantum systems, *SciPost Phys. Codebases* **7** (2022).
- [76] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information: 10th Anniversary Edition* (Cambridge University Press, Cambridge, 2010).
- [77] D. Hofmann, G. Fabiani, J. H. Mentink, G. Carleo, and M. A. Sentef, Role of stochastic noise and generalization error in the time propagation of neural-network quantum states, *SciPost Phys.* **12**, 165 (2022).
- [78] J.-G. Liu, Y.-H. Zhang, Y. Wan, and L. Wang, Variational quantum eigensolver with fewer qubits, *Phys. Rev. Res.* **1**, 023025 (2019).
- [79] S. McArdle, S. Endo, A. Aspuru-Guzik, S. C. Benjamin, and X. Yuan, Quantum computational chemistry, *Rev. Mod. Phys.* **92**, 015003 (2020).
- [80] G. Kotliar, S. Y. Savrasov, K. Haule, V. S. Oudovenko, O. Parcollet, and C. A. Marianetti, Electronic structure calculations with dynamical mean-field theory, *Rev. Mod. Phys.* **78**, 865 (2006).
- [81] Q. Sun and G. K.-L. Chan, Quantum embedding theories, *Acc. Chem. Res.* **49**, 2705 (2016).
- [82] U. Schollwöck, The density-matrix renormalization group in the age of matrix product states, *Ann. Phys.* **326**, 96 (2011), January 2011 Special Issue.
- [83] G. Carleo and M. Troyer, Solving the quantum many-body problem with artificial neural networks, *Science* **355**, 602 (2017).
- [84] R. Mansuroglu, F. Fischer, and M. J. Hartmann, Problem-specific classical optimization of Hamiltonian simulation, *Phys. Rev. Res.* **5**, 043035 (2023).
- [85] C. Mc Keever and M. Lubasch, Classically optimized Hamiltonian simulation, *Phys. Rev. Res.* **5**, 023146 (2023).
- [86] I. N. M. Le, S. Sun, and C. B. Mendl, Riemannian quantum circuit optimization based on matrix product operators, *Quantum* **9**, 1833 (2025).
- [87] G. H. Low and I. L. Chuang, Hamiltonian simulation by qubitization, *Quantum* **3**, 163 (2019).
- [88] G. Gentinetta, F. Metz, and G. Carleo, Code for “Correcting and extending Trotterized quantum many-body dynamics” (2025), <https://github.com/gentinettagian/CQD>.
- [89] J. Bradbury, R. Frostig, P. Hawkins, M. J. Johnson, C. Leary, D. Maclaurin, and S. Wanderman-Milne, JAX: Composable transformations of PYTHON+NumPy programs, 2018, <http://github.com/jax-ml/jax>.
- [90] J. Heek, A. Levskaya, A. Oliver, M. Ritter, B. Rondepierre, A. Steiner, and M. van Zee, FLAX: A neural network library and ecosystem for JAX, 2024, <http://github.com/google/flax>.
- [91] V. Bergholm, *et al.*, PENNYLANE: Automatic differentiation of hybrid quantum-classical computations, *ArXiv:1811.04968*.