Shallow Trotter circuits fulfil error-resilient quantum simulation of imaginary time

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Computing the ground-state properties of quantum many-body systems is a promising application of near-term quantum hardware with a potential impact in many fields. Quantum phase estimation uses deep circuits and is infeasible without fault-tolerant technologies. Many quantum simulation algorithms developed recently work in an inexact and variational manner to exploit the power of shallow circuits. These algorithms rely on the assumption that variational circuits can produce the desired result. Here, we combine quantum Monte Carlo with quantum computing and propose a quasi-exact algorithm for imaginary-time simulation and ground-state computing. Unlike variational algorithms, our algorithm always approaches the exact solution when the Trotter circuit depth increases. Even when the circuit is shallow, our algorithm can yield an accurate ground-state energy. Compared with quantum phase estimation, the conventional quasi-exact algorithm, our algorithm can reduce the Trotter step number by thousands of times. We verify this resilience to Trotterisation errors in numerical simulation of up to 20 qubits and theoretical analysis. Our results demonstrate that non-variational and exact quantum simulation is promising even without a fully fault-tolerant quantum computer.

I. INTRODUCTION

Solving a theoretical model is basic in physics for producing useful predictions. However, many practical models in quantum mechanics are computationally hard. In the 1980s, Richard Feynman conceived a solution to this problem \cite{1}, i.e. “the possibility that there is to be an exact simulation, that the computer will do exactly the same as nature.” This idea is one of the main motivations for developing quantum computing technologies. In the 1990s, Seth Lloyd proposed the Trotterisation algorithm to simulate real time evolution on a quantum computer \cite{2}. Based on real time simulation (RTS), one can solve the ground-state problem with the quantum phase estimation (QPE) algorithm \cite{3, 4}. Trotterisation and QPE are quasi-exact algorithms, in which one can achieve any accuracy at a polynomial cost in time and qubits. It is widely believed that accurately implementing these two algorithms needs a fault-tolerant quantum computer \cite{5–7}, i.e. the ultimate-goal machine that can reduce the probability of logical errors using quantum error correction \cite{8, 9}.

Simulating real time evolution is intrinsic for a quantum computer. In quantum mechanics, real time evolution is a unitary operator. On a quantum Turing machine, one can realise any unitary operator with a sequence of quantum gates \cite{10}. Trotterisation is a specific realisation of the evolution operator according to the Trotter formula. Compared with real time evolution, the ground state draws more attention as it determines properties of many matters, such as nuclei \cite{11}, molecules \cite{12} and condensate matter systems \cite{13, 14}. Ground-state computing (GSC) using QPE depends on an accurate RTS, which prevents its realisation with today’s technologies. This situation is different from classical computing. Some classical algorithms can successfully solve ground states of certain models, for instance, quantum Monte Carlo \cite{11–13} and density-matrix renormalization group \cite{14}. However, their counterparts for generic RTS are inefficient \cite{15, 16}.

This work introduces a quasi-exact quantum algorithm to simulate imaginary time evolution \cite{17} and solve the ground-state problem by sampling random unitary Trotter circuits. We compare three problems, i.e. RTS, imaginary time simulation (ITS) and GSC. Like classical computing, we show that ITS and GSC are more efficient than RTS with the same resources in quantum computing. When the Trotter circuit depth is inadequate for even approximate RTS, it is still possible to obtain an accurate ground-state energy with our algorithm. In recent years, several approaches have been developed for GSC on a near-term quantum machine, including variational quantum eigensolver \cite{18, 19}, constrained quantum-classical Monte Carlo \cite{20}, quantum subspace diagonalisation \cite{21, 22} and ITS with the variational method \cite{23} or local circuit update according to a variational principle \cite{24}. Despite their feasibility with shallow circuits, these approaches depend on trial wavefunctions, and some of them use quantum-classical iterations involving intensive measurements and feedback. Our algorithm overcomes these disadvantages as it is quasi-exact and iteration-free. In comparison to other works on non-variational simulation, such as ITS using non-unitary gates \cite{25, 26} and modified phase estimation using time series analysis techniques \cite{27–31}, we focus on the impact of Trotterisation techniques. We show that our algorithm has a strong resilience to circuit depth, which enables accurate quantum computing using non-variational shallow circuits. Whereas variational algorithms diverge from Feynman’s original conjecture about universal ex-
FIG. 1. (a) Two-time correlation evaluated with Trotterisation. (b) Two-time correlation along the dashed line in (a). (c) Expected value of the Hamiltonian as a function of time. The exact value converges to the ground-state energy when $\beta$ is large. (d) Schematic of the imaginary time simulation algorithm by sampling random Trotter circuits. The sample generator produces time samples according to a distribution determined by $\beta$ and $\tau$. The quantum processor evaluates two-time correlations using Trotter circuits. The Monte Carlo estimator computes the mean of correlations and outputs the final result. (e) Expected value of the Hamiltonian as a function of $E_0$. The minimum value is taken as the result of the ground-state energy. Note that we can use the same set of quantum-computing data to evaluate results of different $E_0$. Curves in (a,b,c,e) are obtained with the ten-spin one-dimensional transverse-field Ising model. We take $\lambda = 1.2$, $T = 3$, $\tau = 2T$ and $N_T = 20$ in (a,b,c,e), $E_0 = E_{\text{ground}}$ in (a,b,c) and $\beta = T$ in (e).

Our results indicate that solving ground states in non-variational quantum computing may be much easier than expected.

II. PROBLEMS AND MODELS

RTS and ITS are to solve Schrödinger equation $\frac{d}{dt}\langle \Psi(t) \rangle = -\eta \hat{H}\langle \Psi(t) \rangle$, where $\eta = i, 1$ correspond to real and imaginary time, respectively. The solution of this equation reads $\langle \Psi(t) \rangle = e^{-\eta \hat{H} t}\langle \Psi(0) \rangle$, where $e^{-\eta \hat{H} t}$ is the time evolution operator. In quantum computing, Schrödinger equation is solved by realising this operator. Without loss of generality, we take $\hat{H} = \hat{H} - E_0 \mathbb{1}$, where $\hat{H}$ is a traceless operator [i.e. $\text{Tr}(\hat{H}) = 0$], $E_0$ is a tunable constant in quantum computing, and $\mathbb{1}$ is the identity operator. GSC is to solve the time-independent Schrödinger equation $\hat{H}|\Psi\rangle = E|\Psi\rangle$ and find the lowest eigenenergy $E_{\text{ground}}$.

We consider three quantum many-body models to benchmark our algorithm: The transverse-field Ising model $\hat{H} = -(2 - \lambda) \sum_{(i,j)} \sigma^x_i \sigma^x_j - \lambda \sum_i \sigma^z_i$, anti-
ferromagnetic Heisenberg model \( \hat{H} = \sum_{(i,j)} \frac{2-\lambda}{2}(\sigma^+_i \sigma^-_j + \sigma^+_j \sigma^-_i) + \lambda \sigma^+_i \sigma^-_i \) and Fermi-Hubbard model \( \hat{H} = -(2 - \lambda) \sum_{(i,j)} \sum_{\alpha=\uparrow,\downarrow}(a^\dagger_i \alpha a_j \alpha + h.c.) + 2\lambda \sum_{i}(2a^\dagger_i \uparrow a_i \downarrow - 1)(2a^\dagger_i \downarrow a_i \uparrow - 1) \) [32]. The transverse-field Ising model undergoes a transition between the ferromagnetic and paramagnetic phases, and its ground state has long-range correlations in the ferromagnetic phase. Unlike the iteration-based ITS [24], our algorithm is not limited to the finite correlation length and works in both phases.

III. REAL TIME SIMULATION

In our algorithm, RTS is a subroutine to evaluate two-time correlations \( \langle O(t',t') \rangle = \langle \Psi(0) | e^{i\hat{H}t'} O e^{-i\hat{H}t} | \Psi(0) \rangle \), where \( O \) is an observable. When \( O = 1, \hat{H} \), correlations have a symmetry \( \langle O(t,t') \rangle = \langle O(t'-t,0) \rangle \). In actual quantum computing, Trotterisation errors break this symmetry as shown in Fig. 1(a). As we will show later, it is crucial for GSC that we directly evaluate two-time correlations rather than evaluate one-time correlations and extrapolate according to the symmetry.

RTS is inaccurate when the Trotter step number \( N_T \) is small. A Trotterisation circuit is formed of a fixed pattern repeated for \( N_T \) times and only produces accurate results when \( N_T \) is large. Otherwise, the error in RTS is significant. As shown in Fig. 1(b), the error in \( \langle \hat{H} \rangle(t,-t) \) is already comparable to the variation of function itself. We quantitatively characterise the accuracy of RTS with the average error \( \epsilon_R \equiv \frac{1}{T} \int_0^T dt |\langle \hat{H} \rangle_T(t,-t) - \langle \hat{H} \rangle_E(t,-t)\rangle \), where \( T \) specifies the time range, and subscripts ‘T’ and ‘E’ denote Trotterisation and exact results, respectively. We have \( \epsilon_R \simeq 1.4 \) for Fig. 1(b).

IV. IMAGINARY TIME SIMULATION

The first result of this work is that we can implement ITS with a small error based on RTS with a large error. In ITS, we compute

\[
\langle O \rangle(\beta) = \frac{\langle \Psi(0) | e^{-\beta \hat{H}} O e^{-\beta \hat{H}} | \Psi(0) \rangle}{\langle \Psi(0) | e^{-2\beta \hat{H}} | \Psi(0) \rangle},
\]

where \( \beta \) is the imaginary time. Fig. 1(c) shows the result of ITS obtained from data of RTS in Fig. 1(b) (in a much larger time range). Unlike RTS, we can find that the error in ITS is negligible compared with the variation of function itself. We define the average error of ITS,

\[
\epsilon_I \equiv \frac{1}{T} \int_0^T d\beta \langle \hat{H} \rangle_T(\beta) - \langle \hat{H} \rangle_E(\beta) \rangle.
\]

We have \( \epsilon_I \simeq 0.062 \) for Fig. 1(c), which is much smaller than \( \epsilon_R \simeq 1.4 \).

ITS is more accurate than RTS. This conclusion holds for various models and parameters in numerical simulation. As shown in Fig. 2, \( \epsilon_I \) is lower than \( \epsilon_R \) by a factor of 10 to 200 in almost all cases, except the Fermi-Hubbard model with \( \lambda = 0.2 \). Later, we will show that GSC is even more accurate than ITS.

V. ALGORITHM

Our algorithm of ITS has three parts as shown in Fig. 1(d). We follow the framework of quantum-circuit Monte Carlo [33] and construct the imaginary time evolution operator in the spirit of a technique in time series analysis [28]. First, a classical computer generates samples \( (t,t') \) according to the distribution \( P(t,t') = C^{-2}|g(t)g(t')| \), where \( g(t) = \frac{1}{\beta^2 e^{\beta t} + 1} e^{-\beta^2 t e^{\beta t}} \) is a product of Lorentz and Gaussian functions, and \( C = \int dt |g(t)| = \ldots \).
VI. GROUND-STATE COMPUTING

An application of ITS is to compute the ground state. In the long-time limit of imaginary time evolution, we have \( \lim_{\beta \to +\infty} \langle \hat{H} \rangle(\beta) = E_{\text{ground}} \) [see Fig. 1(c)], and expected values of other observables are similar. In practice, \( \beta \) is finite, and \( \langle \hat{H} \rangle(\beta) \) is a function of \( E_0 \) because of Trotterisation errors, see Fig. 1(e). We note that we can change \( E_0 \) without redoing quantum computing. By adding a phase \( e^{i(H_0 - E_0)(t-t')} \) to \( \langle O \rangle(t, t') \), we can effectively change \( E_0 \) to \( E_0' \). In this way, we can generate data for \( E_0' \) with \( \langle O \rangle(t, t') \) for \( E_0 \).

We take the minimum value of \( \langle \hat{H} \rangle(\beta) \) as the final result of the ground-state energy. This minimum-energy method is inspired by variational algorithms. Because of the two-time-correlation approach, \( \langle \hat{H} \rangle(\beta) \) obtained with our algorithm is the expected value of \( \hat{H} \) in the state \( \langle \hat{H} \rangle|\Psi(0)\rangle \) up to Trotterisation errors, and we have \( \langle \hat{H} \rangle(\beta) \geq E_{\text{ground}} \). The minimum-energy method boosts the resilience to Trotterisation errors. We find that GSC is more accurate than ITS in almost all cases, as shown in Fig. 2. Compared with RTS, the error in GSC is smaller by a factor of 30 to 10^5 in numerical simulation.

VII. ERROR RESILIENCE

Now, we present the theoretical result that the impact of Trotterisation errors in ITS is smaller than in RTS. We only consider the first-order Trotter formula, and it is similar for other formulas [36, 37]. In Trotterisation, the Hamiltonian is expressed as a summation of simple traceless operators, i.e. \( \hat{H} = \sum_{j=1}^{M} H_j \), and each \( e^{-iH_j t} \) can be straightforwardly realised with elementary quantum gates. We introduce operators \( H_{k+1} = H_j \) for each integer \( k \) corresponding to the \((k+1)\)th Trotter step. In Trotterisation, the operator \( e^{iE_0 t} \mathcal{P}\{e^{-iH_{\text{sum}} t}\} \) is implemented to approximate \( e^{-i\hat{H} t} \), where \( H_{\text{sum}} = \frac{1}{N_T} \sum_j^{N_T} H_j \), and \( \mathcal{P} \) denotes the ordering operation according to the label of \( H_j \): Operators \( H_j \) are sorted from right to left in ascending order. When RTS is realised with Trotterisation, accordingly the operator \( \mathcal{P}\{G(H_{\text{sum}} - E_0) 1\} \) is effectively implemented to approximate \( G(H) \) in ITS. Taking the leading-order (second-order in this case) contribution, the error in RTS is \( e^{iE_0 t} \mathcal{P}\{e^{-iH_{\text{sum}} t}\} - e^{-i\hat{H} t} \simeq -\frac{\beta^2}{2N_T} R_t \), and the error in ITS is

\[
\mathcal{P}\{G(H_{\text{sum}} - E_0) 1\} - G(H) \simeq \frac{\beta^2}{2N_T} R_t
\]  

where \( |\xi| \leq e^{\beta E_0} + e^{-\frac{\beta^2}{2}} \left( 1 + \sqrt{\frac{2\beta}{\pi}} \right) \) and \( R \equiv \sum_{i=1}^{M-1} \sum_{j=i+1}^{M} |H_j, H_i| \).

In RTS, factors \( e^{\beta E_0} \) and \( e^{-\frac{\beta^2}{2}} \) suppress errors. For a traceless Hamiltonian \( \hat{H} \), usually its ground-state energy
$E_{\text{ground}}$ is fairly negative. Therefore, these two exponential factors are small when we take $E_0 \sim E_{\text{ground}}$. Here we only consider the leading-order contribution by applying a truncation on Taylor expansion, but the conclusion holds even when parameters exceed the regime of valid truncation. For example, $\|R\|_{2,3}/N_T > 1$ for models in Fig. 2. The same exponential factors also appear in the first-order expansion with respect to $H_{\text{sum}}$ and $H$. Therefore, they also suppress machine errors that cause deviations in gates $e^{-iHt}$. On ibmq quantum computers, we implement the quantum simulation of a two-spin transverse-field Ising model. Because of the simplicity of the simulated model, we can implement simulation without Trotterisation errors, and all errors are due to machine errors and sampling noise. We find that errors in ITS and GSC are much smaller than in RTS in experiments, for about one order of magnitude on ibm_santiago.

An approach of ITS is the direct Trotter decomposition of the imaginary time evolution operator. An algorithm based on this approach, such as Ref. [24], does not have the resilience to Trotterisation errors. See Appendix E 1 for details.

**VIII. ERROR MITIGATION**

Error mitigation techniques are used to minimise machine errors and algorithmic errors without using error correction codes [38–40]. Focusing on Trotterisation errors, there are two approaches, i.e. the error extrapolation with respect to $N_T$ [41] and the quantum-circuit Monte Carlo with Pauli and rotation gates inserted into the circuit [33]. In this work, we implement quantum subspace expansion (QSE) [40] to reduce the error in GSC as follows. By choosing a set of imaginary times $\{\beta_a | a = 1, 2, \ldots, d\}$, we evaluate matrices $A_{a,b} = \langle 1 | (-i\beta_a, i\beta_a) \rangle$ and $B_{a,b} = \langle H | (-i\beta_a, i\beta_a) \rangle$. Given the unitary diagonalisation $\Lambda = U^\dagger AU$, we have the effective Hamiltonian in the subspace $H_{\text{eff}} = V^\dagger BV$, where $V = UV^\dagger \Lambda^{-1}$. The ground-state energy of $H_{\text{eff}}$ is taken as the error-mitigated result. We can directly evaluate $A$ and $B$ because of the two-time-correlation approach, i.e. we only need to change the distribution $P(t, t')$ according to $\beta_a$ and $\beta_b$. A similar method call quantum Lanczos is proposed in Ref. [24], which is based on one-time correlations. In comparison, the ground-state energy of $H_{\text{eff}}$ obtained from two-time correlations is always greater or equal to the exact $E_{\text{ground}}$, such that we can use the minimum-energy method to find a robust solution. Combining QSE with the minimum-energy method, the error in GSC can be lower than $10^{-7}$ while the error in RTS is $\epsilon_R \sim 1$, as shown in Fig. 2.

**IX. SCALING**

We use the one-dimensional transverse-field Ising model to test the scaling behaviour of our algorithm and infer the impact of Trotterisation errors in hundred-qubit quantum computing. This model demonstrates nontrivial phenomena and has an analytically solvable Hamiltonian [42], i.e. the exact answer is known for any system size. We increase the number of spins $n_{\text{spin}}$ and take the number of Trotter steps $N_T = r n_{\text{spin}}$. The result of numerical simulation shows a trend that the error in the ground-state energy decreases with $n_{\text{spin}}$ when $r$ is a fixed constant, see Fig. 3. Accordingly, considering $N_T = 50$ for $n_{\text{spin}} = 100$, we can infer that the error is smaller than 0.0025, which is much smaller than the energy gap $\sim 0.8$ between the ground and first-excited states.

We note that the accuracy of our algorithm is remarkable considering the small Trotter step number. For $n_{\text{spin}} = 20$ and $N_T = 40$ in Fig. 3, errors in energy are $9.1 \times 10^{-4}$ and $2.8 \times 10^{-5}$ depending on whether QSE is used. To achieve the same energy resolutions using QPE, the conventional quasi-exact algorithm, Trotter step numbers $2.5 \times 10^5$ and $4.6 \times 10^7$ are required, respectively. See Appendix F for details. Therefore, the circuit depth of our algorithm is shallower for thousands to a million times. We further verify this advantage of our algorithm considering GSC of the water molecule. Using QPE, the Trotter step number for achieving the chemical accuracy is about $6 \times 10^5$ [5]; even without QSE, we only need four Trotter steps in our algorithm.

**X. DISCUSSIONS**

Our algorithm is quasi-exact, as the same as Trotterisation of RTS. We can eliminate algorithmic errors with a polynomially increasing circuit depth. This feature is usually absent in variational and variational-like algorithms aiming at the solution in a constrained state subset [18–24]. GSC requires a finite overlap between the initial state and ground state, as the same as QPE [3, 4]. This issue eventually makes the general ground-state problem QMA-hard [43]. In numerical simulation and experiments, we take simple initial states with certain symmetries, such as $|+\rangle^{n_{\text{spin}}}$ in TFI models. Sampling noise is not taken into account in numerical simulation. With sampling noise, the cost for achieving an error as low as $10^{-7}$ is demanding, but it clearly suggests that Trotterisation errors are not an obstacle.

In summary, we can overcome algorithmic errors due to shallow circuits with a proper quantum algorithm design rather than relying on assumptions about variational circuits. In our algorithm, the impact of Trotterisation errors is minimised and sometimes negligible even when the Trotter circuit is shallow. Using a shallow circuit reduces the potential impact of machine errors. In practical quantum computing, specifically in the noisy intermediate-scale quantum era [44], it is crucial to find a trade-off between algorithmic errors and machine errors. The Monte Carlo summation of random circuits as a quantum computing paradigm provides a new dimension to explore to develop efficient quantum algorithms.
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Appendix A: Algorithm

In this section, we discuss the operator $G(H)$, protocols for evaluating $\langle O \rangle (t, t')$ and the Monte Carlo estimator.

1. Integral formula

According to the algorithm, we have

$$G(H) = \int_{-\infty}^{\infty} dtg(t)e^{-iHt}.$$  
(A1)

First, we apply the spectral decomposition to the Hamiltonian, and we get

$$H = \sum_{\omega} \omega |\omega\rangle \langle \omega|,$$  
(A2)

where $\{\omega\}$ are eigenvalues of the Hamiltonian, which are real, and $\{|\omega\rangle\}$ are orthonormal vectors. Then, the real time evolution operator reads

$$e^{-iHt} = \sum_{\omega} e^{-i\omega t} |\omega\rangle \langle \omega|.$$  
(A3)

The integral formula becomes

$$G(H) = \sum_{\omega} G(\omega) |\omega\rangle \langle \omega|,$$  
(A4)

and

$$G(\omega) = \int_{-\infty}^{\infty} dtg(t)e^{-i\omega t}.$$  
(A5)

According to the matrix 2-norm, the error in the integral formula is

$$\|G(H) - e^{-\beta H}\|_2 = \max_{\omega} |G(\omega) - e^{-\beta \omega}|.$$  
(A6)

Here, we have used that

$$e^{-\beta H} = \sum_{\omega} e^{-\beta \omega} |\omega\rangle \langle \omega|.$$  
(A7)

For the Lorentz-Gaussian function, we have

$$G(\omega) = \int_{-\infty}^{\infty} dt \frac{1}{\pi} \frac{\beta}{\beta^2 + t^2} e^{-\frac{\beta^2 + t^2}{2t^2}} e^{-i\omega t}$$

$$= G_+(\omega) + G_-(\omega),$$  
(A8)

where

$$G_\eta(\omega) = \int_{-\infty}^{\infty} dt \frac{1}{\pi} \frac{1}{\pi} e^{-\frac{t^2}{2\eta^2}}.$$  
(A9)

Next, we use the residue theorem to evaluate this integral. We consider the contour in the complex plane $-T + i0 \rightarrow T + i0 \rightarrow T - i\omega T^2 \rightarrow -T - i\omega T^2 \rightarrow -T + i0$, where $T \rightarrow +\infty$.

When $\beta + \eta \omega T^2 > 0$, we have

$$G_\eta(\omega) = e^{-\frac{\beta^2 + \omega^2 t^2}{2t^2}} \int_{-\infty}^{\infty} dt \frac{1}{\pi} e^{-\frac{t^2}{\eta^2}}$$

$$= \frac{1}{2} e^{-\frac{\beta^2 + \omega^2 t^2}{2t^2}} e^{-\frac{\beta \omega T + 1}{\eta^2}}$$

$$= \frac{1}{2} e^{-\frac{\beta \omega T^2}{\eta^2}}.$$  
(A10)

Here, we have used properties of the Faddeeva function. When $\beta + \eta \omega T^2 = 0$, we have

$$G_\eta(\omega) = \frac{1}{2} e^{\eta \omega T} = \frac{1}{2} e^{\eta \omega T^2}.$$  
(A11)

When $\beta + \eta \omega T^2 < 0$, we have

$$G_\eta(\omega) = e^{\eta \omega T} = \frac{1}{2} e^{\eta \omega T^2}.$$  
(A12)

Here, we have used that $\text{erfc}(x) + \text{erfc}(-x) = 2$. Therefore, for all cases, we have

$$G_\eta(\omega) = \frac{1}{2} e^{\eta \omega T^2}.$$  
(A13)

Because $g(t) \geq 0$, the normalisation factor is $C = G(0) = \text{erfc}(\frac{\beta}{\sqrt{2}\eta})$.

To derive the error in the integral formula, we consider $\beta - \omega T^2 < 0$. Using $\text{erfc}(x) \leq e^{-x^2}$ when $x \geq 0$, we have

$$|G(\omega) - e^{-\beta \omega}| \leq \frac{1}{2} e^{\beta \omega} e^{-\frac{(\omega T + 1)^2}{2t^2}} + \frac{1}{2} e^{-\beta \omega} e^{-\frac{(\omega T - 1)^2}{2t^2}}$$

$$= e^{-\frac{\beta^2 + \omega^2 t^2}{2t^2}}.$$  
(A14)

When $\Delta E \geq \frac{\beta}{\tau T}$, we have $\beta - \omega T^2 < 0$ for all $\omega$. Then,

$$\|G(H) - e^{-\beta H}\|_2 \leq e^{-\frac{1}{2}(\Delta E T^2 + \frac{\beta^2}{\tau T})} \leq e^{-\frac{\Delta E T^2}{2T}}.$$  
(A15)

2. Circuit

We propose two protocols for evaluating $\langle O \rangle (t, t')$. One protocol uses an ancillary qubit and works for the general case. The other protocol does not use the ancillary qubit but only works under certain conditions.

The circuit for the ancillary-qubit protocol is shown in Fig. 4. We assume that $O$ is a unitary operator, e.g. a
Pauli operator. For a general operator, we can express it as a linear combination of unitary operators and measure each term. In the circuit, the gate \( U_t \) prepares the initial state, i.e. \( |\Psi(0)\rangle = U_t|0\rangle^\otimes n \). The top qubit is the ancillary qubit, and \( I \) and \( Z \) are Pauli operators acting on the ancillary qubit. The gate \( B \) is for adjusting the measurement basis. Let \( \langle X \rangle \) and \( \langle Y \rangle \) be expected values of ancillary-qubit Pauli operators evaluated using the circuit, then \( \langle O \rangle(t, t') = \langle X \rangle + i\langle Y \rangle \).

The ancillary-qubit-free protocol has three steps: i) Prepare the state \( |\tilde{\Psi}\rangle = \frac{1}{\sqrt{2}}(|\Psi(0)\rangle + |\Psi(1)\rangle) \), where \( |\Psi(0)\rangle \) is a reference state; ii) Apply the transformation \( U = e^{iHt}Oe^{-iHt} \), which is realised with Trotterisation; iii) Measure \( \tilde{X} = |\Psi(0)\rangle\langle \Psi(0) | + |\Psi(1)\rangle\langle \Psi(1) | \) and \( \tilde{Y} = -i|\Psi(0)\rangle\langle \Psi(1) | + i|\Psi(1)\rangle\langle \Psi(0) | \). We have

\[
\text{Tr}\left( \frac{\tilde{X} + i\tilde{Y}}{2} U |\tilde{\Psi}\rangle \langle \tilde{\Psi} | U^\dagger \right)
= \frac{1}{2} \left( \langle \Psi(0) | U |\Psi(0) \rangle + \langle \Psi(1) | U |\Psi(1) \rangle \right)
\times \left( \langle \Psi(0) | U^\dagger |\Psi(0) \rangle + \langle \Psi(1) | U^\dagger |\Psi(1) \rangle \right). \tag{A16}
\]

This protocol works if \( \langle \Psi(0) | U |\Psi(0) \rangle, \langle \Psi(0) | U^\dagger |\Psi(1) \rangle \) and \( \langle \Psi(1) | U^\dagger |\Psi(0) \rangle \) are known. By solving the equation, we can obtain \( \langle \Psi(0) | U |\Psi(0) \rangle \).

For fermion systems with particle number conservation, the ancillary-qubit-free protocol usually works. As proposed in Ref. [35], we can choose the vacuum state as the reference state. In our case, \( U = e^{iHt}Oe^{-iHt} \) is realised with Trotterisation, and we want to take into account algorithmic errors caused by Trotterisation. Therefore, we need to implement Trotterisation in the follow way: We express the Hamiltonian in the summation form \( \hat{H} = \sum_{j=1}^{M} H_j \) for Trotterisation, and each term preserves the particle number. Additionally, it is required that the unitary operator \( O \) preserves the particle number, otherwise we can express it as a linear combination of particle-number-preserving unitary operators and measure each term. Then, we have \( \langle \Psi_i | U |\Psi_i \rangle = e^{i\phi} \), where the phase \( \phi \) usually can be computed analytically. Usually the initial state has non-zero particles, i.e. \( \langle \Psi(0) | \Psi_i \rangle = 0 \), then \( \langle \Psi(0) | U |\Psi_i \rangle = \langle \Psi(0) | U^\dagger |\Psi_i \rangle = 0 \).

3. Monte Carlo estimator

According to the algorithm, we have

\[
\langle O \rangle(-i\beta, i\beta) = C^2 \mathbb{E}[\langle O \rangle(t, t')]
= C^2 \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt' P(t, t') \langle O \rangle(t, t')
= \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt' g(t) g(t') \langle \Psi(0) | e^{iHt}Oe^{-iHt} |\Psi(0) \rangle.
\tag{A17}
\]

Here, we have used that \( g(t) \geq 0 \).

To analyse the variance, we consider the following setup. For each sample \( (t, t') \), the quantum computer implements the circuit in Fig. 4 for one shot and measure the \( X \) operator of the ancillary qubit, which returns a binary number \( \mu_X = \pm 1 \) representing the measurement outcome; and the same circuit is implemented for another shot to measure the \( Y \) operator, which returns \( \mu_Y = \pm 1 \) as the measurement outcome. Then \( \langle O \rangle(-i\beta, i\beta) = C^2 [\mathbb{E}[\mu_X] + i\mathbb{E}[\mu_Y]] \). The variance of the real part is

\[
\text{Var}_R = C^2 \frac{1 - \mathbb{E}[\mu_X]^2}{4N_s} \leq \frac{1}{4N_s}. \tag{A18}
\]

The variance of the imaginary part is

\[
\text{Var}_I = C^2 \frac{1 - \mathbb{E}[\mu_Y]^2}{4N_s} \leq \frac{1}{4N_s}. \tag{A19}
\]

Here, \( N_s \) is the number of samples. Note that \( C = \text{erfc}(-\frac{\beta}{\sqrt{2\pi}}) \leq 1 \).

We can evaluate \( \hat{H} \) by decomposing it as a linear combination of unitary operators, i.e. \( \hat{H} = \sum \alpha_j O_j \). Here, \( \alpha_j \) are coefficients, and \( O_j \) are unitary operators, e.g. Pauli operators. Then, the variance of \( \langle \hat{H} (-i\beta, i\beta) \rangle \) has the upper bound \( \frac{1}{4N_s} \sum_j |\alpha_j|^2 \). As long as \( \sum_j |\alpha_j|^2 \) scales polynomially with the system size, our algorithm is polynomial. Note that usually this polynomial condition holds for local-interaction Hamiltonians.

Appendix B: Trotterisation

In this section, we describe the Trotter formula in detail and discuss Trotterisation errors. We also discuss the resilience to machine errors.

1. Ordering operation

We consider the Hamiltonian expressed in the summation form \( \hat{H} = \sum_{j=1}^{M} H_j \), where \( H_j \) are Hermitian operator. We introduce operators \( H_{k,M+j} = H_j \) for integers \( k \in [0, N_T - 1] \). We use \( \mathcal{P} \) to denote the ordering operation according to the label of operators \( H_j \).
we take $$\beta$$ simulations and $$T \equiv 20$$, FIG. 5. Errors in quantum simulation of randomly generated Hamiltonians. We take $$n_{\text{spin}} = 10$$, $$N_T = 20$$, $$T = 6$$, $$\tau = 2T$$, $$E_0 = E_{\text{ground}}$$ in real and imaginary time simulations and $$\beta = T$$ in ground-state computing. In QSE, we take $$d = 8$$ and $$\beta_0 = \alpha T/d$$. The second-order Trotter formula is used in the simulation.

$$j = 1, 2, \ldots, N_T M$$: For any product of $$H_j$$ operators, the ordering operation is defined as

$$\mathcal{P} \{ H_{j_1} H_{j_2} \cdots H_{j_K} \} \equiv H_{N_T M}^{k_{N_T M}} \cdots H_2^{k_2} H_1^{k_1},$$

where $$K$$ is the total number of operators in the product, and $$k_j = \sum_{j=1}^K \delta_{j,j}$$, is the number of the $$H_j$$ operator in the product.

To define $$\mathcal{P}$$ for a general function of $$H_j$$ operators, we introduce the spectral decomposition of each $$H_j$$, i.e., $$H_j = \sum_{j, \omega_{j,n_j}} \omega_{j,n_j} \Pi_{j,n_j}$$, where $$\Pi_{j,n_j}$$ is the orthogonal projection onto eigenvector of $$H_j$$ with the eigenvalue $$\omega_{j,n_j}$$. We can find that

$$H_{N_T M}^{k_{N_T M}} \cdots H_2^{k_2} H_1^{k_1} = \sum_{n_{1, n_{2}}, \ldots, n_{N_T M}} \omega_{N_T M}^{k_{N_T M}} \cdots \omega_{2}^{k_2} \omega_{1}^{k_1} \times \Pi_{N_T M, n_{N_T M}} \cdots \Pi_{2, n_2} \Pi_{1, n_1}.$$  

Therefore, for a general function, we define the ordering operation as

$$\mathcal{P} \{ f(H_1, H_2, \ldots, H_{N_T M}) \} = \sum_{n_{1, n_{2}, \ldots, n_{N_T M}}} f(\omega_{1,n_1}, \omega_{2,n_2}, \ldots, \omega_{N_T M, n_{N_T M}}) \times \Pi_{N_T M, n_{N_T M}} \cdots \Pi_{2, n_2} \Pi_{1, n_1}.$$  

Note that for an analytic $$f$$, we can also read $$\mathcal{P} \{ f(H_1, H_2, \ldots, H_{N_T M}) \}$$ as applying the ordering operation on each term in the Taylor expansion of $$f(H_1, H_2, \ldots, H_{N_T M})$$.

In Trotterisation, we use $$\mathcal{P} \{ H^k_{\text{sum}} \}$$ to approximate $$\vec{H}^k$$, where

$$H_{\text{sum}} \equiv \frac{1}{N_T} \sum_{j=1}^{N_T M} H_j.$$  

When $$k = 1$$, we have $$\mathcal{P} \{ H_{\text{sum}} \} = \vec{H}$$. When $$k = 2$$, we have

$$\mathcal{P} \{ H^2_{\text{sum}} \} = \sum_{j=1}^{M} H_j^2 + \left(1 + \frac{1}{N_T} \right) \sum_{i=1}^{M-1} \sum_{j=i+1}^{M} H_j H_i$$

$$+ \left(1 - \frac{1}{N_T} \right) \sum_{i=2}^{M} \sum_{j=1}^{i-1} H_j H_i$$

and

$$\vec{H}^2 = \sum_{j=1}^{M} H_j^2 + \sum_{i=1}^{M-1} \sum_{j=i+1}^{M} H_j H_i + \sum_{i=2}^{M} \sum_{j=1}^{i-1} H_j H_i.$$  

Then,

$$\mathcal{P} \{ H^2_{\text{sum}} \} - \vec{H}^2 = \frac{1}{N_T} R,$$

where

$$R \equiv \sum_{i=1}^{M-1} \sum_{j=i+1}^{M} [H_j, H_i].$$  

2. Trotter formula

The first-order Trotter formula reads

$$S_1(t) = e^{-i H_1 t} \cdots e^{-i H_2 t} e^{-i H_1 t}. $$

With $$N_T$$ Trotter steps, we use $$\left[ S_1 \left( \frac{t}{N_T} \right) \right]^{N_T}$$ to approximate $$e^{-i \vec{H} t}$$, and

$$\left[ S_1 \left( \frac{t}{N_T} \right) \right]^{N_T} = e^{-i H_{N_T M} t} \cdots e^{-i H_1 t} e^{-i H_{N_T M} t} \mathcal{P} \{ e^{-i H_{\text{sum}} t} \}.$$  

Using the Taylor expansion, we have

$$e^{-i H t} = 1 - i \vec{H} t - \frac{1}{2} \vec{H}^2 t^2 + O(t^3)$$

and

$$\mathcal{P} \{ e^{-i H_{\text{sum}} t} \} = 1 - i H_{\text{sum}} t - \frac{1}{2} \mathcal{P} \{ H^2_{\text{sum}} \} t^2 + O(t^3).$$  

Taking the leading-order contribution to the error, we have

$$\mathcal{P} \{ e^{-i H_{\text{sum}} t} \} - e^{-i \vec{H} t} \simeq - \frac{t^2}{2N_T} R.$$  

3. Integral of the Trotter formula

According to the spectral decomposition, the product becomes

$$\left[ S_1 \left( \frac{t}{N_T} \right) \right]^{N_T} = \sum_{n_1,n_2,\ldots,n_{N_T}} e^{i\sum_{j=1}^{N_T} \omega_j n_j \frac{t}{N_T}}$$

Because

$$\int_{-\infty}^{\infty} dt e^{iE_0 t} e^{-i\sum_{j=1}^{N_T} \omega_j n_j - E_0} = G \left( \frac{1}{N_T} \sum_{j=1}^{N_T} \omega_j n_j - E_0 \right),$$

we have

$$\int_{-\infty}^{\infty} dt e^{iE_0 t} \left[ S_1 \left( \frac{t}{N_T} \right) \right]^{N_T} = \sum_{n_1,n_2,\ldots,n_{N_T}} G \left( \frac{1}{N_T} \sum_{j=1}^{N_T} \omega_j n_j - E_0 \right) \prod_{n_1,n_2,\ldots,n_{N_T}} \cdot \cdot \cdot \Pi_{n_1,n_2} \Pi_{1,n_1}$$

$$= \mathcal{P} \left\{ G(\sum_{n} E_0) \right\}. \quad (B16)$$

Note that without the Gaussian function, we have $G(\omega) = e^{i\omega^2/2}$, and we cannot obtain the analytic formula for the integral of the Trotter product.

Now, we consider the first- and second-order derivatives of the function $G(\omega)$. We have

$$G'(\omega) = \sum_{\eta=\pm} \frac{\eta \beta}{2} e^{\eta \beta \omega} \text{erfc} \left( \frac{\beta + \eta \omega \tau^2}{\sqrt{2} \tau} \right), \quad (B17)$$

$$G''(\omega) = -e^{-\frac{1}{2} \omega^2 + \frac{\omega^2}{2\tau^2}} \sqrt{\frac{2}{\pi} \tau \beta} + G(\omega) \beta^2. \quad (B18)$$

Similar to Trotterisation errors of the real time simulation, we use the Taylor expansion and take the leading-order contribution to the error. We have

$$\mathcal{P} \{ G(\sum_{n} E_0) \} = G(H) \approx G''(-E_0) \frac{R}{2N_T}. \quad (B19)$$

When $\bar{H}$ is traceless, $E_{\text{ground}}$ is usually negative. Then $-E_0 \sqrt{2/\pi} \geq 0$ when $E_{\text{ground}} - E_0 \geq \frac{\beta}{\tau}$. Under this condition, we have

$$|G''(-E_0)| \leq e^{\beta E_0} e^{-\frac{1}{4} \left( \frac{E_0}{\beta} + \frac{2}{\beta} \right)} \left( 1 + \sqrt{\frac{2}{\tau \beta}} \right) \leq e^{\beta E_0} e^{-\frac{E_0^2}{4}} \left( 1 + \sqrt{\frac{2}{\tau \beta}} \right). \quad (B20)$$

For machine errors, we consider the following error model: Due to imperfection of the machine, each gate $e^{-i\bar{H}_j \frac{t}{N_T}}$ becomes $e^{-i\bar{H}_j \frac{t}{N_T}}$. Then, the transformation realised in quantum computing is $\mathcal{P} \{ G(\sum_{n} E_0) \}$, where

$$H'_{\text{sum}} = \frac{1}{N_T} \sum_{j=1}^{N_T} H_j. \quad (B21)$$

Taking the leading-order contribution to the error, we have

$$\mathcal{P} \{ G(H'_{\text{sum}} - E_0) \} \simeq G''(-E_0)(H'_{\text{sum}} - \bar{H}), \quad (B22)$$

where

$$|G''(-E_0)| \leq \beta \left( e^{\beta E_0} e^{-\frac{E_0^2}{4}} \right). \quad (B23)$$
TABLE I. Error $\epsilon$ and corresponding Trotter step numbers in our quantum-circuit Monte Carlo (QCMC) algorithm [without and with quantum subspace expansion (QSE)] and the quantum phase estimation (QPE) algorithm. Here, we list the result of the one-dimensional transverse-field Ising model with $n_{\text{spin}} = 20$.

| $\epsilon$          | QCMC (raw) | QPE   | $\epsilon$ | QCMC (QSE) | QPE   |
|---------------------|------------|-------|------------|------------|-------|
| $2.0 \times 10^{-2}$| 10         | $2.4 \times 10^3$ | $2.5 \times 10^{-3}$ | 10         | $5.3 \times 10^4$ |
| $5.1 \times 10^{-3}$| 20         | $1.9 \times 10^4$ | $4.6 \times 10^{-4}$ | 20         | $7.0 \times 10^5$ |
| $2.0 \times 10^{-3}$| 30         | $7.9 \times 10^5$ | $9.4 \times 10^{-5}$ | 30         | $7.5 \times 10^6$ |
| $9.1 \times 10^{-4}$| 40         | $2.5 \times 10^6$ | $2.8 \times 10^{-5}$ | 40         | $4.6 \times 10^7$ |

FIG. 7. Error in time evolution operators in the real-time simulation (RTS), imaginary-time simulation (ITS) using direct decomposition and ITS using quantum-circuit Monte Carlo (QCMC). We take $t = \beta = 2$ and $\tau = 2\beta$. $N_T$ is the number of Trotter steps.

Appendix C: Numerics

In this section, we give details of numerical simulation and results of the random Hamiltonian test. Results of the random Hamiltonian test shown in Fig. 5

1. Models

For all three models, we choose the periodic boundary condition: The topology is a ring for one-dimensional models, and the topology is a torus for two-dimensional models. To simulate the Fermi-Hubbard model in quantum computing, we use the Jordan-Wigner transformation to translate the Fermion Hamiltonian into a qubit Hamiltonian [32]. The one-dimensional Fermi-Hubbard model is translated into the qubit Hamiltonian

$$\hat{H} = H_X + H_Y + H_Z,$$  \hspace{1cm} (C1)

where

$$H_X = -\frac{2-\lambda}{2} \left[ \sum_{i=1}^{n_{\text{site}}-1} (\sigma^x_{i+1} + \sigma^x_{i+1}) \right]$$

$$+ \prod_{j=2}^{n_{\text{site}}-1} \sigma^y_j \sigma^y_j$$

$$+ \prod_{j=2}^{n_{\text{site}}-1} \sigma^z_{i+1} \sigma^z_{i+1} + \sigma^z_{i+1} \sigma^z_{i+1} \right],$$  \hspace{1cm} (C2)

$$H_Y = -\frac{2-\lambda}{2} \left[ \sum_{i=1}^{n_{\text{site}}-1} (\sigma^y_i + \sigma^y_i + \sigma^y_i + \sigma^y_i) \right]$$

$$+ \prod_{j=2}^{n_{\text{site}}-1} \sigma^x_j \sigma^x_j$$

$$+ \prod_{j=2}^{n_{\text{site}}-1} \sigma^z_{i+1} \sigma^z_{i+1} + \sigma^z_{i+1} \sigma^z_{i+1} \right],$$  \hspace{1cm} (C3)

$$H_Z = 2\lambda \sum_i \sigma^z_i \sigma^z_i.$$  \hspace{1cm} (C4)

In the random Hamiltonian test, we consider Hamiltonians in the form

$$\hat{H} = -\lambda_0 \sum_{j=1}^{n_{\text{spin}}} \sigma^z_j + \sum_{l=1}^{n_{\text{term}}} \lambda_l \sigma^z_l,$$  \hspace{1cm} (C5)

where $\sigma^z_l \in \{\sigma^z, \sigma^z, \sigma^z, \sigma^z\} \otimes n_{\text{spin}}$ are Pauli operators, where $\sigma^z$ is the identity operator. By taking this Hamiltonian, the spectrum is likely to have a finite energy gap between the ground and first-excited states, and the ground state has a finite overlap with $|0\rangle \otimes n_{\text{spin}}$. The finite gap and overlap are essential for efficient ground-state computing. Without the finite gap, $\langle \hat{H} \rangle/\beta$ converges slowly to the ground-state energy.

We generate $P_l$ in two ways. In the k-local test, we take $P_l = \prod_{j=1}^{n_{\text{spin}}} \sigma^z_j$, and each $\sigma^z_j$ is drawn from $(i, x, y, z)$ with probabilities $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ respectively. Therefore, $k = n_{\text{spin}}/2$ on average. In the 2-local test, we take $P_l = \sigma^z_j \sigma^z_j$, and $\sigma^z_j$ and $\sigma^z_j$ are chosen as follows. When $l \leq n_{\text{spin}} - 1$, we take $j_2 = l + 1$ and randomly choose $j_1$ from numbers smaller than $l + 1$, and each $\alpha$
is drawn from \((x, y)\). In this way, all spins are coupled. When \(l \geq n_{\text{spin}}\), we randomly choose a pair of qubits for \(j_1\) and \(j_2\), and each \(\alpha\) is drawn from \((x, y, z)\).

Parameters \(\lambda\) are taken as follows. We take \(\lambda_0 = 2n_{\text{spin}}/(n_{\text{spin}} + n_{\text{term}})\). Initially, each \(\lambda_i\) is a random number in the range \(-1\) to \(1\); then, \(\lambda_i\) are normalised such that \(\sum_{i=1}^{n_{\text{term}}} |\lambda_i| = 2n_{\text{spin}}/n_{\text{term}} + n_{\text{term}}\). In this way, we have \(n_{\text{spin}}\lambda_0 + \sum_{i=1}^{n_{\text{term}}} |\lambda_i| = 2n_{\text{spin}}\). Note that each term \((\sigma_{\alpha}^z \otimes P)\) in the Hamiltonian has the same strength on average.

2. Details of numerical simulation

In Trotterisation, we decompose the Hamiltonian as follows. For the transverse-field Ising model, we take
\[
H_1 = -(2 - \lambda) \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z \quad \text{and} \quad H_2 = -\lambda \sum_i \sigma_i^z.
\]
For the anti-ferromagnetic Heisenberg model, we take
\[
H_1 = \sum_{\langle i,j \rangle} 2\lambda \sigma_i^x \sigma_j^x, \quad H_2 = \sum_{\langle i,j \rangle} 2\lambda \sigma_i^y \sigma_j^y \quad \text{and} \quad H_3 = \sum_{\langle i,j \rangle} \lambda \sigma_i^z \sigma_j^z.
\]
For the Fermi-Hubbard model, we take
\[
H_l = H_X, \quad H_y = H_Y \quad \text{and} \quad H_Z = H_Z.
\]
In random Hamiltonian test, each \(H_j\) is a Pauli-operator term in the Hamiltonian.

We take the initial state as follows. For the transverse-field Ising model, we take \(|\Psi(0)\rangle = |+\rangle^\otimes n_{\text{spin}}\). For the anti-ferromagnetic Heisenberg model, we take \(|\Psi(0)\rangle = (\frac{1}{\sqrt{2}}(|01\rangle - |10\rangle))^\otimes n_{\text{spin}}\), i.e. each pair of nearest neighboring qubits are initialised in the state with zero total spin. For the Fermi-Hubbard model, we take \(|\Psi(0)\rangle = \prod_{\alpha=1}^{n_{\text{spin}}/2} \left( a_{1\alpha}^\dagger a_{2\alpha}^\dagger + a_{1\alpha} a_{2\alpha} \right) \left| \text{Vac} \right\rangle\), where \(|\text{Vac}\rangle = |0\rangle^\otimes n_{\text{spin}}\) denotes the vacuum state. In random Hamiltonian test, we take \(|\Psi(0)\rangle = |0\rangle^\otimes n_{\text{spin}}\).

In numerical simulation, we neglect machine errors and sampling noise. In the numerical integration, we use the simplest midpoint rule with the step size \(\delta t = T/20\). The numerical integration is truncated at \(\pm 10T\).

To obtain a stable inverse in the numerical calculation, we apply a truncation on eigenvalues of \(A\). We suppose eigenvalues are \(\lambda_1, \lambda_2, \ldots, \lambda_d\) in descending order, and the number of eigenvalues greater than \(\epsilon_0 = 10^{-10}\) is \(d_0\). Then, the inverse matrix \(\sqrt{\Lambda^{-1}}\) is replaced by the \(d_0 \times d_0\) matrix \(\Lambda_{\text{eff}}\) with elements \(\Lambda_{\text{eff}}^{\alpha \beta} = \delta_{\alpha \beta} \sqrt{\lambda_{\text{eff}}^{\alpha \beta}}\). Accordingly, \(H_{\text{eff}}\) is a \(d_0 \times d_0\) matrix.

Appendix D: Experiments

In experiments, we simulate real time evolution using the variational quantum simulation algorithm. We express the state as
\[
|\Psi(t)\rangle = e^{-i\phi(t)(\sigma_1^z \sigma_2^z)} e^{-i\theta(t)(\sigma_1^z \sigma_2^z)} |+\rangle^\otimes 2.
\]

The functions \(\phi(t)\) and \(\theta(t)\) are determined by variational principles as given in Ref. [38]. We can work out \(\phi(t)\) and \(\theta(t)\) in a quantum-classical hybrid manner. For a demonstration, we work out \(\phi(t)\) and \(\theta(t)\) on a classical computer and then use the result in experiments. Because of the simplicity of the simulated Hamiltonian, RTS is exact when machine errors and sampling noise are neglected. Therefore, all errors in experiment are due to machine errors and sampling noise.

On IBM quantum computers, we evaluate correlations \((\langle H \rangle(t, -t)\) and \(\langle \bar{H} \rangle(t, -t)\). We take \(t = -375\delta t, -36\delta t, \ldots, 375\delta t\), where \(\delta t = T/75\), and \(T = \frac{\pi^2}{2}(2 - \lambda^2) + \lambda^2\). For the simulated Hamiltonian, real time evolution is periodic, and \(T\) is the period. Therefore, with the data of one period, we can extrapolate data of other periods. The numerical integration is implemented with the truncation at \(\pm 100T\). General two-time correlations are extrapolated according to their symmetry.

Appendix E: Imaginary-time simulation algorithms

A way to directly simulate imaginary time evolution is constructing the evolution operator \(e^{-\beta H}\) using non-unitary gates. The realisation of non-unitary gates requires measurements for each time step [25, 26]. Ref. [25] reports an explicit algorithm of how to realise non-unitary gates and simulate the imaginary time evolution using elementary quantum gates, however, the complexity is not polynomial.

In comparison, our algorithm is polynomial: 1) The Trotterisation error converges to zero polynomially when the Trotter step number increases; 2) The Monte Carlo calculation is free of the sign problem, and the sampling cost scales polynomially with the required accuracy (i.e. variance), system size and evolution time, see Appendix. A 3.

Another way to simulate imaginary time evolution is approximating the non-unitary evolution operator \(e^{-\beta H}\) using a unitary operator [23, 24]. The unitary operator is determined by searching for the optimal one in a set of operators in a variational manner. One needs to assume that there is a good approximation in the operator set, which is usually formed by those feasible with shallow circuits. It is demonstrated in Ref. [24] that a good approximation exists and can be found if the correlation length in the state is short. These algorithms find the desired operator in quantum-classical iterations, as the same as variational quantum eigensolver.

In addition to manipulating the quantum state, one can simulate imaginary time evolution in a fully classical manner using auxiliary-field quantum Monte Carlo [20]. The algorithm is non-variational but depends on assuming that the trial state is close to the ground state. Otherwise, the constraint on the sign of weights causes a bias (error) in the result.
1. Direct decomposition

The algorithm in Ref. [24] uses a direct Trotter decomposition of the imaginary time evolution operator. The product \( \left[ S_1 \left( -i \frac{t}{N_T} \right) \right]^{N_T} \) is used to approximate the operator \( e^{-\bar{H}t} \). This approach does not have the resilience to Trotterisation errors. To demonstrate the impact of Trotterisation errors, we consider a simple Hamiltonian \( \bar{H} = \sigma^z + \sigma^z \), and we take \( \bar{H} = \bar{H} - E_0 \mathbb{1} \) and \( E_0 = E_{\text{ground}} \), where \( E_{\text{ground}} \) is the ground-state energy of \( \bar{H} \). By taking \( E_0 = E_{\text{ground}} \), we have \( \|e^{-iE_0t}\|_2 = \|e^{-\bar{H}t}\|_2 = 1 \) for all \( t \). In our algorithm, we use Trotterisation and quantum-circuit Monte Carlo to realise the operator \( G(\bar{H}) \). Taking \( \tau = 2\beta \), we have \( \|G(H)\|_2 = 0.6171 \) for all \( \beta \).

We compute errors in time evolution operators in the real-time simulation, imaginary-time simulation using direct decomposition and imaginary-time simulation using quantum-circuit Monte Carlo. The errors are

\[
\left\| e^{iE_0t} \left[ S_1 \left( -i \frac{t}{N_T} \right) \right]^{N_T} - e^{-i\bar{H}t} \right\|_2 ,
\]

and

\[
\left\| e^{E_0t} \left[ S_1 \left( -i \frac{t}{N_T} \right) \right]^{N_T} - e^{-\bar{H}t} \right\|_2 ,
\]

and

\[
\| \mathcal{P} \left( G(H_{\text{sum}} - E_0 \mathbb{1}) \right) - G(H) \|_2 ,
\]

respectively. The result is plotted in Fig. 7. We can find that our quantum-circuit Monte Carlo algorithm is robust to Trotterisation errors, however, the imaginary-time simulation using direct decomposition is even more sensitive to Trotterisation errors than the real-time simulation.

Appendix F: Phase estimation

In this section, we compare Trotter step numbers in two algorithms: our quantum-circuit Monte Carlo algorithm and the phase estimation algorithm. We consider computing the ground-state energy of the one-dimensional transverse-field Ising model with \( \lambda = 1.2 \). The numerical result of our algorithm is shown in Fig. 3 in the main text. When \( n_{\text{spin}} = 20 \), the error in the ground-state energy is \( \epsilon \), which is shown in Table I.

In phase estimation, eigenvalues of a Hamiltonian are estimated by measuring the phase \( e^{-iE_0t} \) due to real time evolution. Here, \( E_0 \) is an eigenvalue, and \( t \) is the evolution time. To achieve the energy resolution \( \epsilon \), the required evolution time is \( t \sim \pi \epsilon^{-1} [5] \), and it is similar for time series analysis [28]. In Trotterisation, the operator \( S_1(\delta t) \) is implemented to approximate the exact time evolution operator \( e^{-i\bar{H}t} \). Therefore, the spectrum of the effective Hamiltonian \( H_{\text{eff}} = \frac{1}{\lambda} \ln S_1(\delta t) \) is actually measured in phase estimation. Then, the error is the difference between ground-state energies of \( H \) and \( H_{\text{eff}} \). By simulating Trotterisation numerically, we obtain the error for varies \( n_{\text{spin}} \) and \( \delta t \), and the results are plotted in Fig. 6. By fitting the data, we find that the error scales with \( n_{\text{spin}} \) and \( \delta t \) in the form

\[ \epsilon = a\delta t^2 \]  \hspace{1cm} (F1)

and

\[ a = 0.228605n_{\text{spin}} + 0.132962. \]  \hspace{1cm} (F2)
Therefore, given $\epsilon$, we take $\delta t = \sqrt{\epsilon / a}$. Then, the Trotter step number is $N_T = t / \delta t = \pi \sqrt{\alpha / \epsilon \sqrt{\epsilon}}$. Now, we can estimate Trotter step numbers in phase estimation. The results are shown in Table 1.

Our algorithm uses fewer Trotter steps to achieve the same accuracy compared with phase estimation. In the comparison, we use the first-order Trotter formula for both algorithms. The advantage of our algorithm is due to i) the resilience of the operator $G(H)$ to Trotterisation errors and ii) the minimum-energy method and quantum subspace expansion used in ground-state computing. The minimum-energy method and quantum subspace expansion can reduce the impact of Trotterisation errors because of the two-time correlation approach utilised in our algorithm.

1. Water molecule

We also observe the advantage of our algorithm in computing the ground-state energy of a molecule. As the same as in Ref. [5], we compute the ground-state energy of the water molecule in a minimal STO-3G basis of 10 electrons in 14 spin orbitals. The Hamiltonian of the water molecule at bond length 0.9584 \AA and bond angle 104.45° is generated and encoded into qubits using qiskit_nature [47]. The unit of energy is hartree ($E_h$). In our algorithm, we take $\beta = 3 E_h^{-1}$ and $\tau = 2\beta$. Both the first- and second-order Trotter formulas are used in our simulation, and results are shown in Fig. 8. We can find that the chemical accuracy (about 1 millihartree) is achieved with $N_T = 4$ using the second-order Trotter formula. We note that the circuit depth is doubled using the second-order formula compared with the first-order formula.

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