Quantum Kernel Function Expansion for Thermal Quantum Ensemble

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Simulating quantum many-body systems is one major application of quantum computing, having a huge potential to impact the fields of computational physics and quantum chemistry. To fulfill the potential impacts, it is crucial to design quantum algorithms that efficiently employ the computation power of the quantum computing devices. Here, we introduce a quantum kernel function expansion algorithm for determining the thermodynamic quantities of quantum many-body systems, including local observables, free energy, and thermal entropy, which has been inspired by the kernel polynomial method in classical Hamiltonian simulation. We design quantum circuits to measure Fourier moments which constitute the thermal ensemble average as an analytic function of energy density via kernel Fourier expansion. Implementing this algorithm on a quantum computer has exponential quantum advantage in the cost of time and space, as compared to its classical analogue. In computing finite temperature properties of a quantum system our quantum algorithm has an overall polynomial time complexity, provided that the corresponding Hamiltonian ground state problem belongs to $\text{BQP}$. We demonstrate its efficiency with applications to one and two-dimensional quantum spin models, and a fermionic lattice. By analyzing the realization on digital and analogue quantum devices, we show the quantum algorithm is accessible to near-term quantum technology.

Introduction.— The computation of thermodynamic quantities of a microscopic quantum Hamiltonian is at the core of simulating correlated electrons in quantum materials and complex molecules [1, 2]. The exponential complexity in treating a large number of entangled degrees of freedom on a classical computer prevents accurate determination of macroscopic physics [3, 4], causing a generic challenge to our quantitative description of a broad range of strongly correlated quantum phases from quantum magnetism [5] and high $T_c$ superconductivity [6] to neutron star matters [7].

With controllable quantum systems, one way that has been carried out is to synthesize analog Hamiltonian models and extract the thermodynamic properties by preparing experimental systems at thermal equilibrium [8–10]. Strongly correlated physics such as Mott-superfluid transition [11, 12], unitary Fermi gas [13], and antiferromagnetism [14–16] have been accomplished with cold atoms. With rapid advancement of programmable quantum devices in the last several years such as superconducting qubits [17–20], trapped ions [21, 22], entangled photons [23–27], and Rydberg atoms [28–31], there have been growing research interests in developing algorithmic approaches for quantum simulations [32–37]. Much progress has been made for determining ground states considering variants of quantum phase estimation [38, 39], adiabatic Hamiltonian evolution [40, 41], and variational quantum circuits [1, 2, 42, 43]. Quantum algorithms for finite temperature quantum simulations have also been proposed using generalized Metropolis sampling [32, 44, 45], quantum Lanczos methods [34], and state filtering [36]. Finite temperature quantum simulation algorithms are relatively scarce as compared to the ground state computation, and efficient computation methods for free energy and thermal entropy, which are crucial for determining thermodynamics, are particularly lacking and in great demand.

In this work, we introduce a quantum kernel function expansion (QKFE) algorithm where the energy dependence of observables and many-body density-of-states (DOS) are represented by Fourier series. We show the expansion moments can be measured by quantum circuits with polynomial cost, achieving an exponential quantum advantage over the classical analogue, namely, the kernel polynomial method (KPM) [46]. The overall complexity of QKFE is exponential in approaching low-temperature properties of a generic Hamiltonian, which is a corollary of Hamiltonian QMA completeness [47–49]. We further develop a thermal ensemble iteration protocol combining QKFE with Hamiltonian evolution, which computes thermodynamical quantities such as local observables, free energy, and thermal entropy with polynomial complexity, provided that determining the ground state of the Hamiltonian belongs to $\text{BQP}$. In our construction, we establish an inherent connection between finite temperature and quantum ground state quantum simulation algorithms.

Quantum kernel function expansion algorithm.— As inspired by the classical KPM algorithm [46], we start by approximating the many-body DOS by Fourier expansion. For a many-body system with Hamiltonian $\hat{H}$,
its DOS is defined by $\rho(E) = \frac{1}{D} \sum_{i} \delta(E - E_i)$, with $E_i$ an eigenvalue of $\hat{H}$, $D = 2^N$ the Hilbert space dimension, $L$ the number of qubits of the system. For convenience in theoretical treatment, we assume the energy spectra are bounded in between $E_{\text{min}}$ and $E_{\text{max}}$, and introduce a dimensionless energy $\varepsilon \equiv (E - E_{\text{min}})/E_w \in [0, 1]$. A rescaled Hamiltonian is introduced as $\hat{H} = (\hat{H} - E_{\text{min}}) / E_w$, correspondingly. This rescaling can always be performed for a lattice Hamiltonian having a finite dimension. The Fourier transform of the DOS takes a form

$$\rho(\varepsilon) = c_0 + 2 \sum_{n=1}^{N-1} c_n \cos(n \pi \varepsilon),$$

with $N$ a high frequency cutoff. The Fourier moments are given by

$$c_n = \frac{1}{2D} \text{Re} \left\{ \text{Tr} \left[ e^{-i \pi \varepsilon \hat{H}} \right] \right\}.$$

This expansion moment can be measured by a quantum circuit shown in Fig. 1(a), which contains $L+1$ number of qubits. The step of averaging $\text{Tr}[\ldots]/D$ is performed by sampling Haar random states [50], whose computation efficiency relies on quantum typicality [51–53]. Despite the difficulty of preparing exact Haar randomness, it can be approximated by relatively shallow circuits [54–57]. The procedure for measuring $c_n$ contains three steps. We choose $R$ number of random product states as the circuit input and scramble these states by performing $\hat{U}_s$ [50]. We then apply the control unitary $|0\rangle \langle 0| \otimes \mathbb{1} + |1\rangle \langle 1| \otimes e^{-i \varepsilon \hat{H}}$ across the ancilla qubit and the system, and take measurements after. The measurement outcomes of $\sigma_y$ on the ancilla qubit average to the $c_n$ moment. This type of observables can also be obtained by quantum nondemolition measurements [58, 59].

For an observable $\hat{A}$, we consider the function $A(\varepsilon) = \langle \varepsilon | \hat{A} | \varepsilon \rangle$, and perform an expansion,

$$A(\varepsilon) \rho(\varepsilon) = d_0 + 2 \sum_{n=1}^{N-1} d_n \cos(n \pi \varepsilon),$$

with the moments

$$d_n = \frac{1}{2D} \text{Re} \left\{ \text{Tr} \left[ e^{-i \varepsilon \hat{H}} \right] \right\}.$$  

These $d_n$ moments can be measured by the same quantum circuit as $c_n$. The measurement outcomes of the $\hat{A}$ operator at the final state of quantum circuit average to the $d_n$ moments.

Having the Fourier moments $c_n$ and $d_n$ measured by quantum circuits, we reconstruct the functions $\rho(\varepsilon)$ and $A(\varepsilon)$, in which the moments are corrected by multiplying a Jackson kernel [50], to damp out the cutoff induced Gibbs oscillations [46]. The resultant function expansion has a uniform convergence with a residual error $O(1/N)$ [50]. The partition function $Z(\beta) = \text{Tr} \left[ e^{-\beta \hat{H}} \right]$ and the canonical ensemble average $A(\beta) = \text{tr} \left[ \hat{A} e^{-\beta \hat{H}} / Z(\beta) \right]$, are then given by

$$Z(\beta) = \int_0^1 e^{-\beta E_w} \rho(\varepsilon) \, d\varepsilon, $$

$$A(\beta) = \frac{1}{Z(\beta)} \int_0^1 e^{-\beta E_w} A(\varepsilon) \rho(\varepsilon) \, d\varepsilon.$$

The QKFE algorithm has close analogue with the classical KPM. In comparing with the classical analogue, the quantum algorithm has an exponential speedup in computing the expansion moments—the time cost for classical KPM is exponential, whereas it is polynomial in
FIG. 2. Finite temperature correlations with the QKFE algorithm. The three panels from top to bottom correspond to 1D-XXZ, 2D-XXZ, and t-V models. For the 1D-XXZ and t-V models, we choose \( R = 20 \) in sampling random states, and for the 2D-XXZ model, we choose \( R = 400 \). The lines represent the numerical results by QKFE. The colored shadows surrounding these lines are sampling errors. The circles show the exact values for comparison.

To benchmark the overall performance of our QKFE, we apply this algorithm to three lattice models including a one-dimensional (1D) spin-1/2 XXZ chain,

\[
\hat{H}_{1D-XXZ} = \sum_j \hat{\sigma}_j^x \hat{\sigma}_{j+1}^x + \hat{\sigma}_j^y \hat{\sigma}_{j+1}^y + \Delta \hat{\sigma}_j^z \hat{\sigma}_{j+1}^z, \tag{5}
\]
a two-dimensional (2D) XXZ model,

\[
\hat{H}_{2D-XXZ} = \sum_{<i,j>} \hat{\sigma}_i^x \hat{\sigma}_j^x + \hat{\sigma}_i^y \hat{\sigma}_j^y + \Delta' \hat{\sigma}_i^z \hat{\sigma}_j^z, \tag{6}
\]
and a 2D t-V model of spinless fermions,

\[
\hat{H}_{tV} = -\sum_{<i,j>} \hat{c}_i^\dagger \hat{c}_j + \hat{c}_i^\dagger \hat{c}_i + V \sum_{<i,j>} \hat{n}_i \hat{n}_j. \tag{7}
\]

In the numerical tests, we choose \( \Delta = -0.9 \), \( \Delta' = -0.5 \), and \( V = 2 \). Since all the three models studied here respect U(1) symmetries, we develop a protocol of generating approximate Haar random states in symmetry-preserving Hilbert space sectors [50]. In Fig. 1, we show the dependence of the expansion moments and partition function on the expansion cutoff \( N \) and the sampling number of random states \( R \) in using QKFE. The convergence is observed at \( R \to 20 \), and \( N \to 100 \).

For local observables, we examine \( C_{1D-XXZ} \equiv \hat{\sigma}_1^z \hat{\sigma}_2^z \), \( C_{2D-XXZ} \equiv \hat{\sigma}_1^z \hat{\sigma}_2^z \), and \( C_{tV} \equiv \hat{n}_{11} \hat{n}_{22} + \hat{n}_{11} \hat{n}_{33} + \hat{n}_{11} \hat{n}_{44} \), for the 1D-XXZ, 2D-XXZ, and t-V models, respectively. We have also checked other observables and find similar behavior as presented here. Fig. 2 shows the performance of QKFE in a broad temperature range. It is apparent that the quantum algorithm performs well in the high temperature regime for all three models. In the low temperature regime, QKFE is no longer reliable, producing substantial computation errors. The large sampling error implies a large number of \( R \) is required at low temperature. The sizable discrepancy between the QKFE and exact calculation indicates a larger cutoff \( N \) is also needed to approximate the functions in Eqs. (2, 4) at low temperature.

The inefficiency of QKFE at low temperature can be attributed to two aspects. First, the low energy states of the many-body Hamiltonian only make an exponentially small contribution to the moments. It is then unavoidable to sample an exponential number \( (R) \) of random states because an exponential precision would be required for the moments. Second, the DOS at low energy is exponentially smaller as compared to high energy. This makes it difficult for the Fourier expansion to approximate the entire energy window. Nonetheless, the exponential speedup in QKFE in computing the moments over the classical KPM remains valid, because these two aspects are also present for classical KPM in simulating low-energy many-body physics. In fact, the exponential time cost for generic low-temperature quantum simulations is a corollary of Hamiltonian QMA completeness [32, 44, 45].

**Thermal ensemble iteration protocol.**—We further develop a polynomial quantum algorithm for a restricted class of Hamiltonian assuming that its ground state determination belongs to BQP [48]. For a Hamiltonian in BQP (\( \hat{H}_{BQP} \)), it is guaranteed that the ground state can be reached by a polynomial quantum circuit, which can be converted to an adiabatic Hamiltonian evolution by introducing clock qubits [41, 60]. The Hamiltonian evolution is denoted as \( \hat{H}_{\text{sys+clock}}(t)|_{t \in [0,T]} \), which involves entangling the system and clock qubits during the time evolution. The adiabatic Hamiltonian path can always be constructed for any initial product state [50].

We choose a product state that gives \( E(\beta = 0) \), with \( E(\beta) \) the thermal ensemble average with respect to \( \hat{H}_{\text{BQP}} \). Such a product state is typical and can thus be efficiently achieved due to the exponential dominance of
infinite-temperature states in the Hilbert space. We let the state evolve under Hamiltonian evolution, i.e., with $U = T_\tau e^{-\beta H_{\text{BQP}}} \mathbb{1}$, and perform a measurement on clock qubits at $t = \tau$, which disentangles the system and the clock qubits. We then replace the Hamiltonian on the system qubits by $\hat{H}_{\text{BQP}}$, and let the system evolve for a certain amount of equilibration time. This procedure produces a ground state on the system qubits if a certain amount of equilibration time. This procedure produces a ground state on the system qubits if $\tau$ reaches the adiabatic limit, say $\tau_{\text{ad}}$, which scales polynomially with the qubit number for BQP. In the limit of $\tau \to 0$, the final state has an energy corresponding to infinite-temperature ensemble average. For the continuity of the energy as a function of $\tau$, the energy of the final states scans through the whole window $[E(\infty), E(0)]$ by varying $\tau$ from 0 to $\tau_{\text{ad}}$. This procedure implies preparing finite energy states is inherently tied to the quantum ground state problem.

To prepare a canonical ensemble, we can prepare multiple $(M)$ copies of $\hat{H}_{\text{BQP}}$, which are allowed to exchange energy by weak interactions. It has been proved that the reduced density matrix of each copy is typically very close to the canonical ensemble, with a trace distance that decays exponentially with $M$ [61]. We remark here that for NISQ devices [62], which unavoidably couple to the environment anyway, preparing multiple copies is unnecessary. By taking measurements on the prepared quantum state, the energy $E$ and local observables $A$ are accessible. But attaining the function $A(\beta)$ or the partition function $Z(\beta)$ requires calculating $\beta(E)$, which cannot be measured directly by the quantum circuit.

Now we develop a thermal ensemble iteration (THEI) protocol for computing $\beta(E)$ based on our QKFE strat-egy. With the prepared canonical ensemble $\hat{\Omega}_\beta = e^{-\beta \hat{H}_{\text{BQP}}} / Z(\beta)$, the Fourier moments as a function of the rescaled average energy $\epsilon_*$. $c_n(\epsilon_*) = \text{Re} \left\{ \text{Tr} \left[ \hat{\Omega}_\beta e^{-\beta \hat{H}_{\text{BQP}}} \right] \right\}$, are measurable by the quantum circuit in Fig. 1. The function $\rho(\epsilon) = e^{-\beta \epsilon} / Z(\beta)$ is then approximated by $G(\epsilon, \epsilon_*) = c_0 + 2 \sum_{n=1}^{N-1} c_n'(n\pi\epsilon)$. Suppose $\beta(\epsilon_*)$ is already known, $\beta(\epsilon_* + \delta_\epsilon)$ is obtained by minimizing the variance of $I(\epsilon) = G(\epsilon, \epsilon_*) - G(\epsilon, \epsilon_* + \delta_\epsilon)$.

The partition function at $\beta = 0$ is trivially given by the Hilbert space dimension $D$, the iteration by Eq. (8) then also produces the partition function $Z(\beta)$, from which the free energy is given by $F(\beta) = -\log Z(\beta)/\beta$, and the thermal entropy is given by $S(\beta) = \beta [E(\beta) - F(\beta)]$, with Boltzman constant taken as a unit.

We apply the THEI protocol to the 1D XXZ model. The results are shown in Fig. 3. It is evident this protocol performs well for the entire temperature range. We confirm the computed inverse temperature, free energy and thermal entropy by the iteration protocol matches on the exact values, with errors barely noticeable.

**Conclusion.** We developed a quantum kernel function expansion algorithm for finite temperature quantum simulations. For a generic Hamiltonian, the QKFE algorithm has an exponential quantum advantage as compared to its classical analogue in computing expansion moments. For a BQP Hamiltonian, we equip QKFE with a THEI protocol, which constitutes an efficient finite temperature quantum simulation method for computing thermodynamic quantities with polynomial time cost.

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Supplementary Materials

S-1. SAMPLING SYMMETRY PRESERVING HAAR RANDOM STATES

In our QKFE algorithm, it is required to evaluate a trace over the Hilbert space, whose computation cost in general scales with the dimension \(D\). But the computation can be performed efficiently with sampling Haar random states, for the sampling variance is bounded by the quantum typicality \([51–53]\),

\[
\begin{align*}
\mathbb{E}_\psi \langle \hat{O} \rangle & = \frac{1}{D} \text{Tr} \left[ \hat{O} \right] \\
\text{Var}_\psi \langle \hat{O} \rangle & = \frac{1}{D+1} \left( \text{Tr} \left[ \hat{O}^2 \right] / D - \left( \text{Tr} \left[ \hat{O} \right] \right)^2 / D^2 \right) 
\end{align*}
\]  

(S1)

with \(\psi\) a Haar random state. In our calculation, we prepare Haar random states by applying a relatively shallow quantum circuits on random product states, which has been shown to produce high-quality approximation for Haar randomness \([54–57]\). In the circuit shown in Fig. 1 (a), we adopt the protocol in Ref. 57, where the unitary \(U_i\) has \(d\) cycles. There are one layer of single-qubit gates and one layer of two-qubit gates in each circle. The single-qubit gates are randomly chosen from the gate-set \(\{X, Y, T\}\) and two-qubit gates are fixed to be C-Z gates.

![Circuit Diagram](image)

FIG. S1. Scheme for sampling U(1) symmetry preserving random states. (a), The illustration of sampling circuit. (b), The entropy \(S_p(|\psi_k\rangle)\) approaches the random state values at moderate layer parameter \(k\) for symmetry sectors with total spin \(S_z = 0, 1, 2\). (c). Correlation results of QKFE algorithm using symmetry preserving sampling for 1D-XXZ model with \(R = 20\) and \(N = 100\). Red circles are respective ED results. In (b) and (c), the shadows surround the lines show error bar for each setting.

Since there is a broad range of Hamiltonian models having U(1) symmetry, for example, spin XXZ models, and Hubbard models, we propose a scheme for sampling U(1) symmetry preserving Haar random states here. The corresponding quantum circuit is shown in Fig. S1. This circuit still involves cycles of gates, with one cycle containing two layers. In the first layer of one cycle, instead of performing single-qubit gates, which in general breaks U(1) symmetry,
we act a unitary $U(t_k) = e^{iHt_k}$ with the corresponding Hamiltonian respecting U(1) symmetry. The time interval $t_k$ is randomly chosen. In the second layer, we still apply C-Z gates, which preserves the U(1) symmetry. Fig. S1 shows the results for the 1D XXZ model. The input state should be some bit-string product state $|\psi_{in}\rangle$ in a certain symmetry sector. To characterize how well this scheme reaches Haar randomness, we examine an entropy $S_{p}(\{|\psi_k\rangle\}) = - \sum p_i \ln p_i$ with $p_i = |c_i|^2$ [57], $c_i$ the wave function in the computation basis (Fig. S1(b)). This entropy measures the spreading in the computational basis of the quantum state after $k$ cycles ($|\psi_k\rangle$). For a $L$-qubit system, $S_{p_k}$ of a true Haar random state is $\log(2L) - 1 + \gamma$, with $\gamma$ the Euler constant, $\approx 0.577$. With our proposed symmetry preserving quantum circuit, we observe $S_{p_k}$ quickly saturates to the ideal value within about 25 cycles, which has been found for different symmetry sectors. This indicates U(1) symmetry preserving Haar random states have indeed been achieved. Fig. S1(c) shows the correlation results for the 1D XXZ model (see the main text). With $R = 20$, and $N = 100$, we find a nice agreement of QKFE algorithm with the exact results.

The physical intuition behind our proposed scheme for preparing symmetry preserving Haar randomness is to let the system thermalize at infinite temperature in a specific symmetry sector—we scramble the system by $U(t_k)$ and destroy energy conservation by the C-Z gates. We expect this approach can be readily generalized to other symmetries.

### S-2. UNIFORM CONVERGENCE IN KERNEL FOURIER EXPANSION

It is well-known that to approximate an analytic function $F(\varepsilon)$, the Fourier series expansion

$$F_N(\varepsilon) = c_0 + 2 \sum_{n=1}^{N-1} c_n \cos(n\pi\varepsilon)$$

has an exponential convergence. However, if $F(\varepsilon)$ is only continuous, uniform convergence is not guaranteed. The Fourier series expansion may potentially suffer from finite $N$ induced Gibbs oscillations. In order to reach uniform convergence, we need to apply kernel functions to the Fourier expansion.

For a continuous function $f(x)$ with $x \in (-1, 1)$, it has been shown in classical KPM analysis [46] that the $N$-th order Chebyshev expansion

$$f_N(x) = \tilde{c}_0 + 2 \sum_{n=1}^{N-1} \tilde{c}_n T_n(x)$$  \hspace{1cm} (S2)$$

has a uniform convergence to $f(x)$, with

$$\tilde{c}_n = h_n \int_{-1}^{1} f(x) T_n(x) \frac{dx}{\pi \sqrt{1 - x^2}}$$

$$h_n = \frac{(N - n + 1) \cos \frac{\pi n}{N+1} + \sin \frac{\pi n}{N+1} \cot \frac{\pi}{N+1}}{N+1},$$

$$T_n(x) = \cos(n \arccos(x)),$$

where $h_n$ is Jackson Kernel [63]. Approximating $f(x)$ by $f_N(x)$ has an error [46],

$$||f(x) - f_N(x)||_\infty \sim w_f(1/N),$$  \hspace{1cm} (S3)$$

with $w_f(\delta) = \max|f(x) - f(y)|_{|x-y|\leq\delta}$. This can be interpreted as an error at the order of $O(1/N)$.

The Fourier expansion used in our work is related to the Chebyshev expansion by taking $x = \cos(n\pi\varepsilon)$, and $F(\varepsilon) = f(\cos(n\pi\varepsilon))$. For $\varepsilon \in (0, 1)$, we have $T_n(x) = \cos(n\pi\varepsilon)$. It follows immediately from Eq. (S3) that $||F(\varepsilon) - f_N(\cos(n\pi\varepsilon))||_\infty \sim w_f(1/N)$, with

$$f_N(\cos(n\pi\varepsilon)) = \tilde{c}_0 + 2 \sum_{n=1}^{N-1} \tilde{c}_n \cos(n\pi\varepsilon),$$
\[ c_n = h_n \int_0^1 F(\epsilon) \cos(n\pi \epsilon) d\epsilon. \]

We thus conclude the kernel Fourier series expansion has uniform convergence with error \( O(1/N) \).

S-3. HAMILTONIAN EVOLUTION SCHEME FOR PREPARING CANONICAL ENSEMBLE

Since it has been proved that a subsystem of a pure state with finite energy density is exponentially close to a canonical ensemble description [61], the key to prepare canonical ensemble is to prepare a finite energy state. Here, we provide two Hamiltonian evolution schemes for this purpose.

To prepare a finite energy state of \( \hat{H}_{\text{BQP}} \), one straightforward approach is to start from a trivial Hamiltonian \( \hat{H}_0 = \sum_i h_i \hat{\sigma}_i^z \), and continuously evolve the system following a time-dependent Hamiltonian,

\[ H(t) = \left( 1 - \left( \frac{t}{\tau} \right) \right) \hat{H}_0 + \left( \frac{t}{\tau} \right) \hat{H}_{\text{BQP}}. \]

One remark is if \( \hat{H}_0 \) and \( \hat{H}_{\text{BQP}} \) happen to commute, we then need to add extra quantum fluctuations by introducing auxiliary Hamiltonians. This is analogous to the adiabatic quantum computing, except that the time evolution is not necessarily adiabatic. The system is initialized at the ground state of \( \hat{H}_0 \) at \( t = 0 \). We choose the configuration of \( h_i \), such that the initial state has an energy \( E(\beta = 0) \), corresponding to the infinite temperature ensemble, with respect to \( \hat{H}_{\text{BQP}} \). Such a state is typical in randomly sampling the product states, as the density of states is exponentially dominant at the \( E(\beta = 0) \) by central limit theorem. In the adiabatic limit with \( \tau \to \tau_{\text{ad}} \) (\( \tau_{\text{ad}} \) a required time scale to reach adiabaticity), a quantum ground state is prepared, having an energy \( E(\beta = +\infty) \). By decreasing \( \tau \) away from the adiabatic limit, the energy of the final state would tend to increase, and in the limit of \( \tau \to 0 \), we necessarily have a quantum state having an energy \( E(\beta = 0) \). By varying \( \tau \) continuously from 0 to \( \tau_{\text{ad}} \), the energy of states prepared by the Hamiltonian evolution procedure necessarily cover \([E(\beta = +\infty), E(\beta = 0)]\) for continuity. This scheme is easy to implement in the experiment, and is expected to be efficient for physical systems in absence of disorder, provided there is no first order transition in Hamiltonian evolution. However, the problem with this scheme is that it is difficult to prove the efficiency rigorously.

The second approach we present here is by introducing auxiliary clock qubits [41, 60]. This approach is less straightforward for experimental implementation, but can be proved to have polynomial time cost. We still start from the same initial product state as described above. Since the Hamiltonian we consider here belongs to BQP, there must be a polynomial-depth quantum circuit that converts the initial product state to the ground state of \( \hat{H}_{\text{BQP}} \). Denoting the computation history as

\[ |\alpha(k)\rangle = U_k |\alpha(k-1)\rangle, \]

with \( k \) labeling the computation steps from 1 to \( d \) (\( d \) is the circuit depth), and \( U_k \) is the applied local unitary at \( k \)-th step. Introducing \( d \) number of auxiliary clock qubits, we define composite states

\[ |\gamma(k)\rangle = |\alpha(k)\rangle_{\text{sys}} \otimes |1^k0^{d-k}\rangle_{\text{clock}}. \]

It has been shown in Refs. 41 and 60 that one can construct a Hamiltonian \( \hat{H}_{\text{final}} \) whose ground state is

\[ |\Psi\rangle = \frac{1}{\sqrt{d+1}} \sum_k |\gamma(k)\rangle. \quad (S4) \]

The Hamiltonian evolution takes a form of

\[ \hat{H}_{\text{sys} \times \text{clock}}(t) = \left( 1 - \left( \frac{t}{\tau} \right) \right) \hat{H}_{\text{init}} + \left( \frac{t}{\tau} \right) \hat{H}_{\text{final}}, \quad (S5) \]
with the initial Hamiltonian containing three parts \( H_{\text{init}} = H_{\text{clock init}} + H_{\text{input}} + H_{\text{clock}} \),

\[
H_{\text{clock init}} = \sum_k (\sigma_k^x + 1),
\]

\[
H_{\text{input}} = \left[ \sum_i h_i (\sigma_i^z + 1) \right] \otimes |0\rangle\langle 0|,
\]

\[
H_{\text{clock}} = \mathbb{1} \otimes \sum_k |01\rangle\langle 01|_{k,k+1}.
\]

Here, \( \sigma \) and \( \delta \) operators act on the physical and clock qubits, respectively. It has been shown that the required evolution time \( \tau_{\text{ad}} \) for reaching the adiabaticity scales polynomially with \( d \) and \( L \) \([12, 41]\). Once the final state is prepared, we take measurements on the clock qubits. The time evolution and the measurement step are repeated until the measurement outcome gives \( |1\rangle \). Then we replace the Hamiltonian on the system by \( H_{\text{BQP}} \). This whole procedure then produces a final state at energy \( E(\beta = 0) \) and \( E(\beta = +\infty) \), in the two limits of \( \tau \to 0 \) and \( \tau \to \tau_{\text{ad}} \), just like the first approach. One remark is that although the constructed Hamiltonians, \( H_{\text{init}} \) and \( H_{\text{final}} \), are not local, a local construction can be performed as well by introducing geometric clock states \([41, 64]\).

### S-4. PHYSICAL REALIZATION AND QUANTUM CIRCUIT COMPLEXITY

One key building block for our quantum algorithms is the control-unitary. In this section we discuss its physical realization, considering both digital quantum circuits and analogue quantum simulation setups, and analyze the resource cost.

#### A. Digital quantum circuits

In digital quantum computation, it is crucial to know how the number multi-partite quantum gates scale with the system size. We take the 1D transverse field Ising (TFI) model for illustration. The time cost scaling is similar for other spin models. The Hamiltonian for the TFI model reads as,

\[
\tilde{H} = \sum_{i=1}^{L-1} \sigma_i^z \sigma_{i+1}^z - \Delta \sum_{j=1}^L \sigma_j^x.
\]

Now suppose the evolution time is \( m\pi \), consider the following Trotter decomposition with a time step \( \delta \)

\[
e^{-im\pi \tilde{H}} = \left[ \prod_{j=1}^{L-1} e^{-i\delta (\sigma_j^z \sigma_{j+1}^z)} \right]^{n} \mathcal{O}(\delta^2),
\]

(S6)

where \( n = m\pi\delta^{-1} \). By gate decomposition, in terms of multi-qubit gates, realization of a controlled-\( e^{i\delta \Delta \sigma_i^z} \) gate needs two CNOT gates, while a controlled-\( e^{-i\delta (\sigma_j^z \sigma_{j+1}^z)} \) gate needs two Toffoli gates and two CNOT gates. Based on the decomposition in Eq. (S6), the number of CNOT gates is \((4L - 2)m\pi\delta^{-1}\), and the number of Toffoli gates is \(2(L - 1)(\delta^{-1})m\pi\delta^{-1}\), for digital realization of the control unitaries. For a finite expansion order \( N \), the overall computation of QKFE algorithm requires \( N \) times of running quantum circuits with depth \( O(NL\delta^{-1}) \). This is reasonably accessible to near-term quantum technology.

#### B. Analog quantum simulator

Here we take the 1D-XXZ model as an example and consider the ultracold atoms confined in a periodic optical lattice. The atoms are prepared in two hyperfine states with the Zeeman sublevels representing two spin-1/2 states. In the Mott
insulator regime, the system is described by an effective XXZ Hamiltonian \[65\]
\[H = \sum_{\langle ij \rangle} \left[ J_{xy} (S_i^x S_j^x + S_i^y S_j^y) + J_z S_i^z S_j^z \right], \tag{S7}\]
where the spin coupling are mediated by superexchange. We have \( J_{xy} = -4J_0^2 / U_{\uparrow \downarrow} \) and \( J_z = 4J_0^2 / U_{\uparrow \downarrow} - (4J_0^2 / U_{\uparrow \uparrow} + 4J_0^2 / U_{\downarrow \downarrow}) \) with \( J_0 \) the single-particle tunneling across nearby lattice sites, \( U_{\sigma \sigma'} \) the onsite Hubbard interactions. For the one-dimension lattice, the anisotropy in 1-D XXZ Hamiltonian in main text, \( \Delta = J_z / J_{xy} \) is tunable through Feshbach resonance.

To extend the spin coupling to the controllable regime, we adopt the configuration of tilted lattice and Raman-induced tunneling in Refs. 66 and 67. In this case, the linear tilt should be large enough to suppress direct atomic tunnelings. The Raman assisted tunneling is then introduced by setting the Raman detuning \( \delta \omega \) resonant with the energy offset of nearby lattice sites. Specially, we use the Rydberg state as the assist state for Raman transition. With an ancillary qubit which has strong Rydberg blockade effect with all system qubits, the control-unitary operation in Fig.1 in main text can be realized. Such Rydberg-assisted Raman process can be established in principle since single-photon transition to Rydberg state has been realized for alkaline atoms [68, 69].

S-5. THE STEPPING COMPLEXITY IN THE THEI PROTOCOL

In the thermal ensemble iteration (THEI) protocol, thermodynamic quantities are computed by an iteration from high to low temperature. Here we discuss how the iteration steps scales with the system size.

From the uniform convergence of our Fourier series expansion (Section S-2), the function \( \rho(\varepsilon) e^{-\beta \varepsilon} / Z(\beta) \) is well approximated by the expansion \( G(\varepsilon, \varepsilon_*) \) in the energy window \( [\varepsilon_* - \sigma_\varepsilon, \varepsilon_* + \sigma_\varepsilon] \), with \( \sigma_\varepsilon \) the energy fluctuation (rescaled by \( E_w \) in our notation) in the canonical ensemble that scales with the system size as \( 1/\sqrt{L} \) [70]. Within this window both the absolute and relative errors are suppressed by \( O(1/N) \), whereas outside this energy window, the expanded function can be exponentially small, and the relative error is no longer controllable. This sets a requirement on the stepping in the THEI protocol— the step in \( \varepsilon_* \), \( \delta_\varepsilon \) should scale with \( \sigma_\varepsilon \). Computing a thermodynamic quantity as a function of \( \beta \) using THEI involves \( O(\sqrt{L}) \) runs of QKFE. The overall complexity is then \( O(N^2L^{3/2} \delta_t^{-1}) \), with \( \delta_t \) the Trotter step.