Letter

Quadratic acceleration of multistep probabilistic algorithms for state preparation

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Quantum state preparation is a fundamental building block for various problems on a quantum computer. A nonunitary operator is typically designed to decay unwanted states contained in an initial state using ancilla qubits and a probabilistically action. In this Letter, we clarify that this probabilistic nature is a drag for quantum advantages: The probabilistic algorithms do not accelerate the computational process compared to classical ones. Combining quantum amplitude amplification (QAA) with multistep probabilistic algorithms is proposed to address this drawback, achieving quadratic acceleration and quantum advantages. We also find that the multistep probabilistic method with QAA exhibits advantages over quantum phase estimation in terms of infidelity. We also demonstrate it to confirm the quadratic acceleration, using a probabilistic imaginary-time evolution method as an example.

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Introduction. The accurate and efficient calculation of ground states is of considerable importance in the field of quantum physics because it provides key insights into the properties and behavior of diverse quantum systems. Quantum phase estimation (QPE) [1–4] is a promising quantum algorithm that estimates the eigenvalues of input eigenvectors of a Hamiltonian more efficiently than classical computers. Despite the advantages of QPE, the preparation of an input state as close as possible to the ground state remains a problem. If the input state of the QPE contains only a small portion of the ground state, the probability of obtaining the ground-state energy decreases, as indicated by the scaling $O(|c_1|^2)$, where $|c_1|^2$ denotes the weight of the ground state in the input state. Thus, significant research has been conducted on quantum algorithms for ground-state preparation [5–18].

State-preparation schemes based on nonunitary operations have been proposed to obtain the ground state [12–18]. Previous studies have realized imaginary-time evolution (ITE) operators [13,14,17,18], cosine functions [12,15], and shifted step functions [10,11] on quantum computers using ancilla qubits and a probabilistic method, both of which rely on forward- and backward-controlled real-time evolution (CRTE) operators. The implementation of real-time evolution (RTE) operators on quantum computers has been well established in the context of Hamiltonian simulations based on the Trotter decomposition [19–23], Taylor series [24,25], and qubitization [26–29]. Thus, any sophisticated implementation of RTE operators can be incorporated into state-preparation schemes using nonunitary quantum circuits.

The computational costs of quantum algorithms that implement nonunitary operators probabilistically have also been estimated for the cosine function [9,12,15] and ITE operators [30]. These quantum algorithms incur $O(|c_1|^{-2})$ computational costs to obtain the ground state. In particular, if $|c_1| = 1/\sqrt{N}$, where $N = 2^n$ and n denotes the number of qubits, i.e., in a scenario where even the approximate ground state is not known, at least $O(N)$ computational cost is incurred. This implies that quantum acceleration is not realized. The complexity class of ground-state preparation is known to be quantum Merlin-Arthur [31–33]. This fact means that polynomial acceleration for ground-state preparation is the limit for quantum computers. The development of quantum algorithms that exhibit polynomial acceleration is an important research topic. In this Letter, we propose a multistep quantum algorithm that achieves quadratic acceleration of the probabilistic state preparation scheme. The proposed quantum algorithm utilizes quantum amplitude amplification (QAA), which enhances the probability of obtaining a desired state based on repeated operations. First, we summarize quantum algorithms for probabilistic formalisms to implement nonunitary operators and estimate their computational costs. We highlight that existing probabilistic algorithms have a computational scaling of order $O(|c_1|^{-2})$ for state preparation, which compromises quantum advantages. Subsequently, we propose quantum algorithms to achieve quadratic acceleration.

Ground-state preparation. Let us consider a nonunitary operator $f(\mathcal{H})$, where $\mathcal{H}$ is an n-qubit system Hamiltonian. $f(\mathcal{H})$ is embedded in the extended unitary matrix by introducing an ancilla qubit as follows,

$$\mathcal{U} \equiv \begin{pmatrix} f(\mathcal{H}) & \sqrt{1-f^2(\mathcal{H})} \\ \sqrt{1-f^2(\mathcal{H})} & -f(\mathcal{H}) \end{pmatrix}, \tag{1}$$

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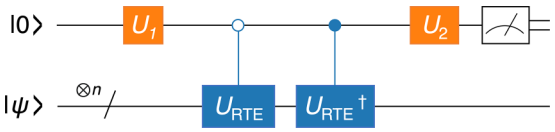

FIG. 1. Quantum circuit of probabilistic algorithm for ground-state preparation. The circuit is composed of a single ancilla qubit and forward and backward CRTE gates. $U_{\mathrm{RTE}} \equiv U_{\mathrm{RTE}}(\Delta\tau) = e^{-i\Delta\tau\mathcal{H}}$ is used in this figure.

comprising submatrices coupled with the ancillary $|0\rangle$ and $|1\rangle$ states. The desired state is obtained when the ancilla is $|0\rangle$, whereas a state coupled to $|1\rangle$ is undesirable. In particular, the action of the unitary matrix $\mathcal{U}$ on the input state leads to

$$f(\mathcal{H})|\psi\rangle \otimes |0\rangle + \sqrt{1 - f^2(\mathcal{H})}|\psi\rangle \otimes |1\rangle. \tag{2}$$

Any unitary matrix $\mathcal{U}$ can be decomposed into at least the first order of $\mathcal{H}$ [see details in Supplemental Material (SM) [34]] and implemented using forward and backward CRTE operations and single-qubit gates (Fig. 1).

During repeated operation, $\mathcal{U}$ involves certain parameters, such as the real time-step size $\Delta\tau$ depicted in Fig. 1, which can be selected freely at each step. The unitary matrix $\mathcal{U}$ at the kth step is denoted by $\mathcal{U}_k$. When K ancilla qubits are used, with a different one used for each $\mathcal{U}_k$ without measuring them, the actions of $\{\mathcal{U}_k\}$ on the input state with the initialized ancilla qubits yield

$$F_K(\mathcal{H})|\psi\rangle \otimes |0\rangle^{\otimes K} + (\text{other states}), \tag{3}$$

where $F_K(\mathcal{H}) \equiv \prod_{k=1}^{K} f_k(\mathcal{H})$. The use of only one ancilla qubit is permitted if we reuse it based on the previous step after measuring and initializing it. $f_k(\mathcal{H})$ was used as an approximate ITE operator $e^{-\Delta\tau_k\mathcal{H}}$ in Ref. [14] and a cosine function $\cos(t_k\mathcal{H})$ in Ref. [12]. Specific quantum circuits are summarized in SM [34]. Repeated operations of $f_k(\mathcal{H})$ decay undesirable states, such as excited states. Quantum signal processing is another approach to design such decay functions [27], where the shifted step function is approximated using a Chebyshev polynomial and implemented using a single ancilla qubit [10,11].

Observing all ancilla qubits in $|0\rangle$ state leads to the collapse of the entangled wave function to

$$|\Psi_K\rangle = \frac{1}{\sqrt{P_K}} F_K(\mathcal{H})|\psi\rangle, \tag{4}$$

where P_K denotes the total probability of all steps being successful. The input state is expanded as follows, $|\psi\rangle = \sum_{i=1}^{N} c_i|\lambda_i\rangle$, where $|\lambda_i\rangle$ denotes the ith eigenstate of the Hamiltonian $\mathcal{H}$ and c_i denotes the expansion coefficient. For simplicity, we assume a nondegenerate and ascending order of eigenvalues; however, the generalization is straightforward. If $F_K(\mathcal{H})$ is well designed to decay the undesired state, then the total success probability becomes

$$P_K = \frac{1}{1 - \delta_K}|c_1|^2, \tag{5}$$

where δ_K denotes the infidelity, defined as $\delta_K \equiv 1 - \mathcal{F}_K$, with fidelity $\mathcal{F}_K \equiv |\langle\lambda_1|\Psi_K\rangle|^2$ (for further details, see SM [34]). Here, we assume $F_K(\lambda_1) = 1$, which is realized by a constant energy shift in the probabilistic imaginary-time evolution (PITE) [30]. Every quantum algorithm that decays the undesirable state to achieve a small value of δ_K using a nonunitary operation exhibits $O(|c_1|^2)$ scaling of the total success probability. Importantly, this implies that the scaling of the total success probability is independent of the type of nonunitary operator $f_k(\mathcal{H})$, the number of ancilla qubits, or the circuit implementation method for $f_k(\mathcal{H})$. If the approximate ground state is not known, e.g., $|c_i|^2 = 1/N$ for each i, the computational cost of at least one success scale is of the order $O(N)$. No quantum acceleration is observed in these algorithms. In contrast, CRTE gates are efficiently implemented at polynomial cost [19–29]. For example, the circuit depth for CRTE for an n_e-electron system based on the first quantization Hamiltonian scales with the order of $d_{\mathrm{CRTE}} = O\{rn_e^2\,\mathrm{poly}[\log(n_e^{1/3}/\Delta x)]\}$, where Δx represents the grid spacing of the discretized space, and r denotes the Trotter number dividing the imaginary-time step size [14,21]. Then, the computational cost is given by

$$\frac{d_{\mathrm{CRTE}}K}{P_K} = O\left[\frac{d_{\mathrm{CRTE}}}{|c_1|^2}\ln\left(\frac{(1-\delta_K)(1-|c_1|^2)}{\delta_K|c_1|^2}\right)\right] \tag{6}$$

(for details, see SM [34]).

Quantum amplitude amplification. Quantum acceleration of ground-state preparation may also be realized using probabilistic algorithms by introducing a multistep scheme and combining it with QAA [29,35–37]. We consider a K-step probabilistic quantum circuit with K ancilla qubits. Each ancilla qubit corresponds to a step of the probabilistic algorithm, and all ancilla qubits are measured after the final step. The output state immediately preceding the measurement is of the form

$$|\widetilde{\Psi}\rangle = a|\Psi_{\mathrm{good}}\rangle + \sqrt{1-a}|\Psi_{\mathrm{bad}}\rangle, \tag{7}$$

where

$$|\Psi_{\mathrm{good}}\rangle = \frac{1}{\sqrt{P_K}} F_k(\mathcal{H})|\psi\rangle \otimes |0\rangle^{\otimes K} \tag{8}$$

is the desired state with weight a and $|\Psi_{\mathrm{bad}}\rangle$ denotes the orthogonal state of $|\Psi_{\mathrm{good}}\rangle$. Owing to introducing the delayed measurement, QAA enhances the coefficients of the $|\Psi_{\mathrm{good}}\rangle$ state by the m-times action $\prod_{i=1}^{m} Q(\phi_{2i-1}, \phi_{2i})$ of the following amplitude amplification operator,

$$Q(\phi_{2i-1}, \phi_{2i}) \equiv -\mathcal{U}_{\mathrm{REF}}^{(K)} S_0^{(n+K)}(\phi_{2i-1}) \left(\mathcal{U}_{\mathrm{REF}}^{(K)}\right)^\dagger S_\chi(\phi_{2i}),$$

where S_χ denotes an oracle, S_0 denotes a zero reflection, and $\mathcal{U}_{\mathrm{REF}}^{(K)}$ is defined as $\mathcal{U}_{\mathrm{REF}}^{(K)}|0\rangle^{\otimes(n+K)} = |\widetilde{\Psi}\rangle$. The rotation angles $\{\phi_i\}$ are chosen as $\phi_i = \pm\pi$ following the conventional method [35,36]; however, recently, approaches have been proposed to determine $\{\phi_i\}$ such that the increase in success probability is an approximated sign function [29,37]. The zero reflection and oracle rotate the output state $|\widetilde{\Psi}\rangle$ in the effective two-dimensional space spanned by $|\Psi_{\mathrm{good}}\rangle$ and $|\Psi_{\mathrm{bad}}\rangle$, which are represented by $S_0^{(n)}(\phi) = e^{i\phi|0\rangle\langle 0|^{\otimes n}}$ and $S_\chi(\phi) = I_{2^n} \otimes S_0^{(K)}(\phi)$, respectively. The circuit depth of the zero-reflection scales at the order of $O(n)$ with a single ancilla qubit [38], and Maslov's gate reduces the scaling preconstant [39]. Figure 2 illustrates the amplitude amplification operator

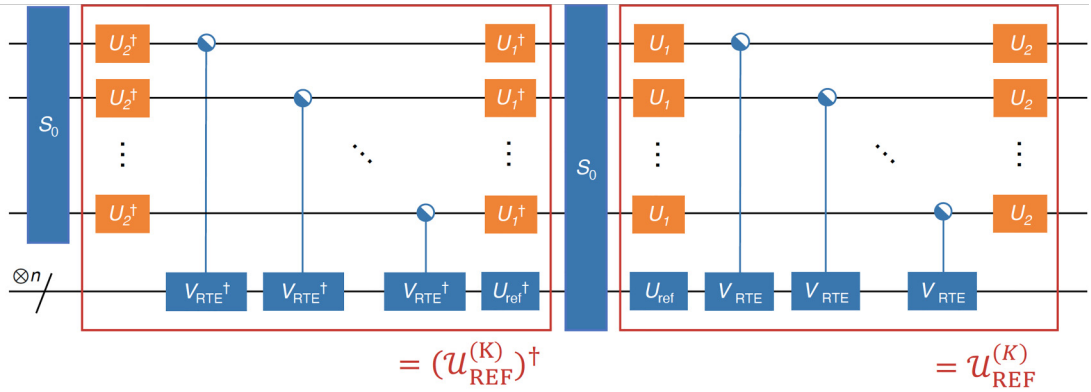

FIG. 2. Quantum circuit for the amplitude amplification operator of the probabilistic algorithm for ground-state preparation given by Eq. (9) while ignoring the global phase. The forward and backward CRTE gates are combined and represented by the controlled-V_{RTE} gate. On the left, S_0 represents $S_0^{(K)}(\phi_{2i})$, while that on the right represents $S_0^{(n+K)}(\phi_{2i-1})$. U_{ref} is defined as $U_{\mathrm{ref}}|0\rangle^{\otimes n} \equiv |\psi\rangle$, which is the input state before the PITE circuit. In the red box on the right, $V_{\mathrm{RTE}} = V_{\mathrm{RTE}}(t_1)$, $V_{\mathrm{RTE}} = V_{\mathrm{RTE}}(t_2)$, …, $V_{\mathrm{RTE}} = V_{\mathrm{RTE}}(t_K)$ from the left, and $U_1 = U_1^{(1)}$, $U_1 = U_1^{(2)}$, …, $U_1 = U_1^{(K)}$ from the top, where $U_1^{(k)}$ is equal to U_1 in the kth step. The same comments apply to U_2.

Q for the probabilistic algorithm for state preparation in K steps.

The optimal number of repetitions of QAA is derived as follows:

$$m^* = \left\lfloor \frac{(2n+1)\pi}{4\sin^{-1} a} \right\rfloor. \tag{9}$$

Thus, when the total success probability P_K is low, we execute a first-order Taylor expansion for $\sin^{-1} a$ and obtain the order of optimal repetitions, m^*, as $m^* = O(1/|c_1|)$. Accordingly, the computational cost of PITE combined with QAA (henceforth referred to as multistep PITE) is estimated as follows,

$$d_{\mathrm{CRTE}} K m^* = O\left[\frac{d_{\mathrm{CRTE}}}{|c_1|} \ln\left(\frac{(1-\delta_K)(1-|c_1|^2)}{\delta_K |c_1|^2}\right)\right], \tag{10}$$

where the QAA technique achieves a quadratic acceleration by Eq. (6). We also discuss the combined technique comprising PITE and QAA discussed in Ref. [40], where a short-depth circuit is proposed for the first-step PITE and circuit construction is designed for K steps using an ancilla qubit. The multistep PITE method proposed in this Letter is a natural extension of that in Ref. [40] and clearly achieves quadratic acceleration for the whole PITE process.

Quantum phase estimation. QPE is a standard building block, which not only estimates the ground-state energy but also prepares the ground state. Before comparing multistep PITE with QPE in terms of numerical results, we briefly discuss QPE. QPE based on quantum Fourier transform (QFT) achieves Heisenberg scaling. Although it typically requires many ancilla qubits, reusing ancilla qubits after measurement and executing subsequent operations depending on the observations enables the same estimation as that using a single ancilla qubit [4,41–43]. For simplicity, standard QPE based on QFT is considered here. After each execution of QPE, one of the eigenenergies is loaded onto the ancilla qubits in a binary representation. We assume the input state for the QPE is $|\psi\rangle = \sum_{i=1}^N c_i|\lambda_i\rangle$ and K ancilla qubits are used. Using QPE, all eigenvalues $\{\lambda_i\}$, which are assumed to be in ascending order, are expressed by a binary representation $\{k_i\}$. In a realistic situation with a finite number of available ancilla qubits, different eigenvalues $\{\lambda_i\}$ that are energetically close to each other and within an energy resolution $1/T$ can be mapped to the same binary representation k_i, where $T \equiv 2^K$. When we observe k as a binary representation of the estimated eigenvalue, the input state collapses to

$$|\Psi_{\mathrm{QFT}}\rangle = \frac{1}{\sqrt{P_k}} \sum_{i=1}^N c_i \alpha_{k|i} |\lambda_i\rangle, \tag{11}$$

where the state is normalized with probability $P_k = \sum_{i=1}^N |c_i|^2 |\alpha_{k|i}|^2$ and periodic function $\alpha_{k|i}$ is defined as $\alpha_{k|i} \equiv (1/T)\sum_{\tau=0}^{T-1} e^{2\pi i \tau(\lambda_i t_0 - k)/T}$. Here, t_0 is a scaling parameter used to increase or decrease the eigenvalues for precise measurement. By $T \equiv 2^K$, we conclude that the number of ancilla qubits used is directly proportional to the fineness of the resolution of the eigenvalues. Thus, we take $t_0 = 2^{K-N_C}$, where $N_C = \lfloor \log_2(\lambda_N - \lambda_1) \rfloor$. Because the number of queries to CRTE increases exponentially, the computational cost for QPE to obtain the ground-state eigenvalue is given by $O[1/(\sqrt{\delta_K}|c_1|^2)]$ [9,34]. By comparing it with Eq. (6), we emphasize that PITE improves computational cost exponentially with respect to the infidelity δ_K over QPE.

Numerical results. The numerical simulation demonstrates the strengths of the proposed method, which is implemented using QISKIT, an open-source library for quantum simulations [44]. The Heisenberg model is adopted as the computational model,

$$\mathcal{H} = \sum_{\langle j,k \rangle} \vec{\sigma}_j \cdot \vec{\sigma}_k + \sum_j h_j \sigma_j, \tag{12}$$

where $\vec{\sigma}_j = (\sigma_j^x, \sigma_j^y, \sigma_j^z)$ is the Pauli matrix acting on the jth spin and $\langle j, k \rangle$ represents the combination of the nearest neighbors of the closed one-dimensional chain. h_j represents the strength of the magnetic field, which is randomly selected from a uniform distribution $h_j \in [-1, 1]$. The CRTE gate is implemented using a fourth-order Trotter decomposition [45] for even-odd groups of the Hamiltonian [22,23]. The dependence of the accuracy and total computational complexity on the order of the Trotter decomposition is numerically demonstrated in SM [34]. The multistep PITE method is

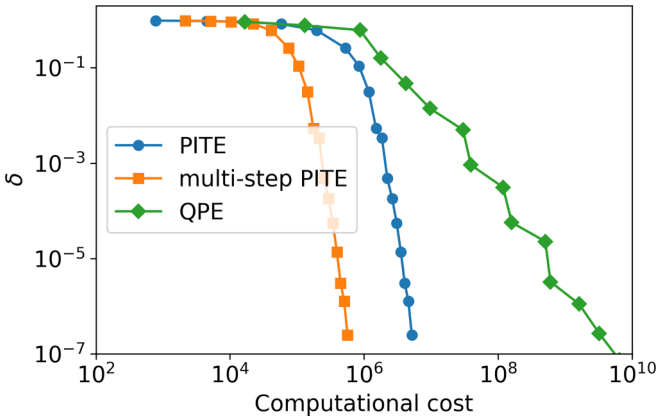

FIG. 3. Plots of the infidelity δ_K as a function of computational cost for PITE, multistep PITE, and QPE, respectively. The results are obtained using the one-dimensional Heisenberg chain with eight spins.

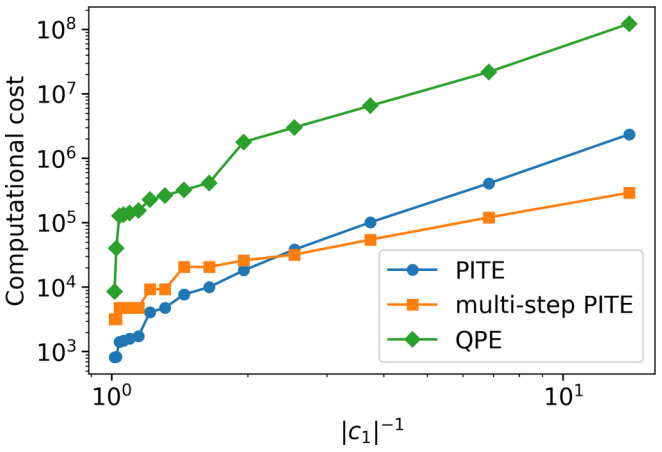

FIG. 4. Plots of computational cost for PITE, multistep PITE, and QPE as functions of the inverse probability weight of the ground state in the input state.

adopted as the probabilistic algorithm while preparing the ground state. The PITE method employs a constant energy shift to increase the total success probability, and adopts computationally efficient scheduling of the imaginary-time step size [30].

Figure 3 illustrates the infidelity δ_K as a function of the computational costs for QPE, PITE, and multistep PITE. The initial state is selected as a uniform probability weight with respect to each eigenvector, i.e., $|c_i|^2 = 1/N$. As the number of steps in PITE or the number of digits, i.e., the resolution in QPE increases, the infidelity decreases, whereas the computational cost increases. As the infidelity decreases, the success probability decreases and approaches $1/N$. This behavior is common in PITE and QPE. PITE and QPE differ in the number of queries in the CRTE block. In QPE, the number of queries increases exponentially with the number of ancilla qubits; thus, the computational cost increases linearly with infidelity. However, in PITE, the number of queries increases linearly with the step, implying that the scaling of the computational cost is logarithmic with respect to infidelity. The figure confirms that PITE is exponentially faster than QPE with respect to infidelity δ_K, as given by Eq. (6). Further, in the case of multistep PITE, we observe an increase in the computational cost due to the quadratic acceleration with respect to the success probability, despite the overhead incurred due to zero reflections. We verify the method with different orders and use a fourth-order Trotter, which yields results in good agreement with the exact solution [34].

To demonstrate quadratic acceleration with respect to the probability weight $|c_1|^2$ of the ground state clearly in the case of multistep PITE, the dependence of computational cost on $|c_1|^2$ is plotted in Fig. 4. The computational cost is estimated when the infidelity is below $\delta_K = 10^{-4}$. The probability weight of the initial state is determined using a Gaussian distribution as a function of the eigenvalues corresponding to the mean ground-state energy. The probability weights of the ground states are increased by changing the variance of the Gaussian distribution. The computational cost of PITE is observed to be lower than that of QPE over the entire region, owing to the exponential advantage of PITE in terms of the infidelity, δ_K. Although the computational cost of multistep PITE is higher than that of PITE without QAA at $|c_1| \approx 1/2$ because of the overhead induced by QAA, it decreases as $|c_1|^{-1}$ increases when $|c_1| < 1/2$. This confirms quadratic acceleration induced by QAA. The crossing point of the computational costs of PITE and multistep PITE is determined by the relationship between the circuit depths of PITE and zero reflection [34]. As the computational overhead induced by zero reflection decreases, QAA increases the computational cost over a wide range.

Conclusions. In this Letter, we propose a quantum algorithm for ground-state preparation that offers several quantum advantages. The recently proposed PITE method, comprising a single ancilla qubit and forward and backward CRTE operations, calculates the ground state nonvariationally on a quantum computer. Although PITE exhibits an exponential advantage over QPE in terms of the infidelity δ, its probabilistic nature degrades the computational cost by a scale of order $O(|c_1|^{-2} \log \delta^{-1})$, where $|c_1|^2$ denotes the probability weight of the ground state in the initial state. Here, we combine QAA with PITE, achieving quadratic acceleration compared to the classical method, where delayed measurement enables multistep amplitude amplification. Numerical simulations emphasize the strengths of the proposed algorithm, which is implemented on a fault-tolerant quantum computer (FTQC). However, the development of quantum algorithms for early FTQC and post-noisy intermediate-scale quantum devices remains an important research topic. In this context, reducing the number of ancilla qubits and the circuit depth of the proposed algorithm is a promising direction for future research. Quantum acceleration beyond quadratic acceleration is a challenging research subject. In addition, preparing a good initial state using classical preprocessing techniques is expected to contribute to fast quantum-state preparation irrespective of the application of QAA. By combining the proposed algorithm, various physical quantities such as the one-body Green's function [46], the linear response function [47], and microcanonical and canonical properties [48] can be calculated. This method is also applicable to various problems such as the optimization of the

structure geometry based on an exhaustive search [49] and investigating an electron under a magnetic field [50]. Thus, this study contributes to the gamut of numerical simulations related to material sciences that are executable on quantum computers.

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[34] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevResearch.6.L022041 for details of the implementation of the nonunitary operators, the derivation of the computational cost for QPE and PITE, and details of the numerical results.

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