Quantum algorithm for calculation of transition amplitudes in hybrid tensor networks

Shu Kanno,† Suguru Endo,‡,§ Yasunari Suzuki,‡,§ and Yuuki Tokunaga‡

1Department of Materials Science and Engineering, Tokyo Institute of Technology, 2-12-1 O-okayama, Meguro-ku, Tokyo 152-8552, Japan
2NTT Secure Platform Laboratories, NTT Corporation, Musashino 180-8585, Japan
3JST, PRESTO, 4-1-8 Honcho, Kawaguchi, Saitama, 332-0012, Japan

The hybrid tensor network approach allows us to perform calculations on systems larger than the scale of a quantum computer. However, when calculating transition amplitudes, there is a problem that the number of terms to be measured increases exponentially with that of the contracted operators. The problem is caused by the fact that the contracted operators are represented as non-Hermitian operators. In this study, we propose a method for the hybrid tensor network calculation that contracts non-Hermitian operators without an exponential increase in the number of terms. In the proposed method, transition amplitudes are calculated by combining the singular value decomposition of the contracted non-Hermitian operators with a Hadamard test. The method significantly extends the applicability of the hybrid tensor network approach.

I. INTRODUCTION

Quantum computers are expected to be capable of executing classically intractable calculations [1–8]. It has been reported that quantum computers can outperform classical computers in some tasks [9–11]. However, quantum resource limitations are obstacles to the practical application of quantum computers. Current quantum computers are so-called noisy intermediate-scale quantum (NISQ) devices [12], and we can control only tens to hundreds of noisy qubits on them [1] [13–18]. Their hardware limitation makes it difficult to apply quantum computers to practical tasks that require large numbers of qubits or deep quantum circuits [19–31].

The hybrid tensor network approach has recently been proposed to overcome the limitations of NISQ devices [19]. The approach enables the treatment of a larger number of quantum states than the number of qubits of actual quantum devices by representing quantum states as a combination of conventional classical tensors and quantum tensors. A quantum tensor has upper and lower indices, for example, $\psi_{j_1,j_2,...,j_L}$, which represents $K$-qubit systems indexed by an $L$-bit string. In other words, the quantum state is defined in terms of $L$ classical bits $(j_1, j_2, \ldots, j_L)$ as

$$|\psi_{j_1,j_2,...,j_L}\rangle = \sum_{i_1,i_2,...,i_K} \psi_{i_1,i_2,...,i_K} |i_1i_2...i_K\rangle,$$  \hspace{1cm} (1)

where $\psi_{j_1,j_2,...,j_L} \in \mathbb{C}$, $\sum_{i_1,i_2,...,i_K} |\psi_{i_1,i_2,...,i_K}|^2 = 1$, and $|i_1i_2...i_K\rangle$ is a computational basis of the $K$-qubit Hilbert space. One of the most vital forms of the hybrid tensor network is the hybrid tree-tensor network, where a network of quantum and classical tensors composes a tree graph. While contraction of general hybrid tensor networks can be costly, hybrid tree-tensor networks can be contracted efficiently to obtain expectation values [19]. In this paper, we mainly discuss a two-layer hybrid tree-tensor network with only quantum tensors, which is called a quantum-quantum tree-tensor network, since it captures the essential properties of hybrid tree-tensor networks and the use of classical tensors restricts the range of representation to classically tractable quantum states such as matrix product states [32]. A quantum-quantum tree-tensor network that expresses $k$ subsystems of $n$-qubit states is represented as

$$|\psi_{HT}\rangle = \sum_{i_1,i_2,...,i_k} \psi_{i_1,i_2,...,i_k} |\varphi^{i_1}\rangle \otimes |\varphi^{i_2}\rangle \otimes \cdots \otimes |\varphi^{i_k}\rangle,$$  \hspace{1cm} (2)

where $|\psi_{HT}\rangle$ is the unnormalized state, $\psi_{i_1,i_2,...,i_k} = \langle i_1i_2...i_k|\psi\rangle$ is the probability amplitude of a $k$-qubit state $|\psi\rangle$, and $|\varphi^{i_m}\rangle (m = 1, 2, \ldots, k)$ is an $n$-qubit state of the $m$-th subsystem indexed by a classical bit $i_m$. Figure 1 shows the network diagram of $|\psi_{HT}\rangle$. While the state $|\psi_{HT}\rangle$ represents a $kn$-qubit state, we can efficiently calculate the expectation value of an observable $O = \bigotimes_{m=1}^{k} O_m$, where $O_m$ operates on $|\varphi^{i_m}\rangle$ via proper tensor contractions, using a quantum computer with $O(\max(k, n))$ qubits. The contraction for evaluating the expectation value $\langle O \rangle = \langle \psi_{HT}|O|\psi_{HT}\rangle$ (without normalization) can be implemented as follows. First, we measure $O_m$ with multiple states and construct operators $M_{m}^{i_m} = \langle \varphi^{i_m}|O_m|\varphi^{i_m}\rangle$. Note that each $M_m$ is a $2 \times 2$ Hermitian matrix when $O_m$ is Hermitian. Then, since $M_m$ is Hermitian, we can measure the expectation value of $\bigotimes_{m=1}^{k} M_m$ for the state $|\psi\rangle$, which is equal to $\langle O \rangle$.

The approach allows for simulations beyond the scale of the quantum hardware. For example, the energy and spin-spin correlation functions of electrons can be calculated with this approach. However, the approach has a serious problem preventing it from being used in a range of applications: it can only calculate the expectation

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* kanno.s.ac@m.titech.ac.jp
† suguru.endou.ac@hco.ntt.co.jp
‡ suguru.endou.ac@hco.ntt.co.jp
§ suguru.endou.ac@hco.ntt.co.jp
value of observables. In other words, there is a problem in the approach when the contracted operator $M_m$ is non-Hermitian. Hereinafter, we denote the Hermitian and non-Hermitian contracted operators as $M_m$ and $N_m$, respectively. The reason for the problem is that the number of terms to be measured increases exponentially with $k$ when $\bigotimes_{m=1}^{k} N_m$ is calculated naively. Specifically, non-Hermitian operators are decomposed into sums of Pauli operators, as in $\bigotimes_{m=1}^{k} N_m = \bigotimes_{m=1}^{k}(h_{1m}I_m + h_{Xm}X_m + h_{Ym}Y_m + h_{Zm}Z_m)$, where $I_m$ is the identity operator, $X_m$, $Y_m$, and $Z_m$ are Pauli operators which act on the $m$-th qubit, and $h_\alpha (\alpha \in \{I, X, Y, Z\})$ are the corresponding coefficients, with up to $4^k$ terms appearing. One example where the problem occurs is in the calculation of the transition amplitude related to Green’s functions and photon emissions/absorptions [33][34]. Overlap of two quantum states, which is exploited in subroutines in many algorithms [33][34], is a special case of the transition amplitude. Thus, the difficulty of computing the expectation value of a non-Hermitian operator limits the applicability of the hybrid tensor network approach.

In this study, we propose a method for calculating transition amplitudes with the hybrid tensor network approach. The main point of the method is the treatment of tensor products of non-Hermitian operators. In a naive calculation, an exponential number of terms in $\bigotimes_{m=1}^{k} N_m$ will appear. We propose two ways to avoid the problem. One is a Monte-Carlo contraction method and the other is a singular value decomposition (SVD) contraction method, and the second method is the main proposal in this paper. Although the first method can avoid having to measure all the terms whose number increases exponentially with $k$, the second method is exponentially more efficient than the first one in terms of the sampling cost.

In the following, we give an overview of quantum-quantum tree-tensor networks [19] for obtaining the expectation values of observables in Sec. IV. Then, the method of calculating transition amplitudes and overlaps is described in Sec. III. The contraction of quantum tensors in subsystems is discussed in Sec. III A and the contraction of non-Hermitian matrices in Sec. III B. We discuss the future applications of the method in Sec. IV.

II. OVERVIEW OF THE HYBRID TENSOR NETWORK

We present an overview of the hybrid tensor network simulation on the state described by Eq. (2) introduced in Ref. [19]. Letting the observable $O$ be $O = \bigotimes_{r=1}^{k} O_r$, and $O_m = \bigotimes_{r=1}^{m} O_{mr} (r = 1, 2, \ldots, n)$, the expectation value of the observable including the normalization constant can be described as

$$
\langle O \rangle = \frac{1}{A^2} \langle \psi_{HT} | O | \psi_{HT} \rangle
$$

and

$$
A = \sqrt{\langle \psi_{HT} | \psi_{HT} \rangle} = \sqrt{\sum_i \bar{\psi}_i^* \psi_i \prod_{m=1}^{k} M_{Am}^{i_m}}
$$

where $A$ is a normalization constant, $\bar{i} = (i_1, i_2, \ldots, i_k)$ with $i_m$ taking either 0 or 1, $M_{Am}^{i_m} = \langle \varphi_{i_m}^m | O_m | \varphi_{i_m}^m \rangle$, and $M_{Am}^{i_m} = \langle \varphi_{i_m}^m | \varphi_{i_m}^m \rangle$. $M_{Am}^{i_m}$ ($M_{Am}^{i_m}$) is an element of the $2 \times 2$ matrix $M_m$ ($M_{Am}$). When $O_m$ is assumed to be an observable, i.e., a Hermitian operator, $M_m$ also becomes a Hermitian operator. $M_{Am}$ is a Hermitian operator since $M_{Am}$ is a special case of $O_m = I_m$ in $M_m$, where $I_m$ is the identity operator.

The procedure for constructing $M_m$ and $M_{Am}$ depends on how the indices $i_m$ of the wave function $|\varphi_{i_m}^m\rangle$ are mapped. We suppose there are two cases of the mapping: one case is where the indices $i_m$ are mapped to unitary gates, i.e., $|\varphi_{i_m}^m\rangle = U_{Cm}^i |0\rangle_\otimes^m$; the other case is where the indices $i_m$ are mapped to the initial wave function $|\varphi_{i_m}^m\rangle = U_{Cm}^i |0\rangle_\otimes^{m-1}$, where $U_{Cm}$ and $U_{Cm}$ are unitary operators with polynomial depth in the $m$-th subsystem. The second case can be regarded as a special example of the first case, since $|\varphi_{i_m}^m\rangle = U_{Cm}^i |m\rangle_\otimes^{m-1} = U_{Cm}(X_1)^i |0\rangle_\otimes^m$ and we can think of $U_{Cm}(X_1)^i |0\rangle_\otimes^m$ as $U_{Cm}(X_1)^i |0\rangle_\otimes^m$, where $X_1$ is a Pauli X operator which acts on the first qubit. Note that the first method needs a Hadamard test circuit while $M_m$ and $M_{Am}$ can be efficiently constructed via direct measurements in the second case, as will be described later.

First, we consider the construction of $M_m$ in the case of $|\varphi_{i_m}^m\rangle = U_{Cm}^i |0\rangle_\otimes^m$. Since the procedure for measuring the diagonal elements is relatively straightforward,
we will focus on the measurement of the non-diagonal elements. Figure 2(a) shows a quantum circuit to obtain the matrix element $M_m^{i,m}$. The procedure for constructing $M_m$ is as follows. First, we prepare initial states.

We use a Hadamard test to prepare $|\phi^m\rangle = U_m^{Cm} |0\rangle^{\otimes n}$ and $|\phi^{*m}\rangle = U_m^{Cm} |0\rangle^{\otimes n}$. The ancilla qubit is initialized to $|0\rangle + e^{i\pi/2}|1\rangle$, where $\alpha$ is the phase. We set $\alpha = 0$ ($\alpha = \frac{\pi}{2}$) to obtain the real (imaginary) part of $M_m^{i,m}$. Since $M_m$ is a Hermitian matrix, only measurements of $\text{Re}(M_m^{i,m})$, and $\text{Im}(M_m^{i,m})$ are required. Then, we measure on a computational basis. We use the fact that $|D\rangle$ noting $D$ is a diagonal matrix. Also, we assign elements of $D$ to the measurement results. More concretely, denoting $D_{mr} = \text{diag}[\lambda_{r=0}^{(mr)}, \lambda_{r=1}^{(mr)}]$, the measured value is computed as $\prod_{r=1}^n \lambda_r^{(mr)}$, corresponding to the measured outcome $j = (j_1, j_2, \ldots, j_n)$.

We explain how to construct $A_m$. Figure 2(b) shows the circuit to construct $A_m$. In the case of $|\phi^m\rangle = U_m^{Cm} |i_m\rangle |0\rangle^{\otimes n-1}$, since the $|\phi^m\rangle$ are non-orthogonal to each other, we have $A \neq 1$. Therefore, $A_m$ must be calculated. The circuit in Fig. 2(b) is a modified version of that in Fig. 2(a), except that system measurements are not necessary; we can construct $A_m$ by using the same construction procedure as for $M_m$.

Next, we assume the case of $|\phi^m\rangle = U_m^{Cm} |i_m\rangle |0\rangle^{\otimes n-1}$. In this case, we can obtain all the elements of $M_m$ only from the results of direct measurements. Figure 2(c) shows a quantum circuit to construct $M_m$. The initial states are set to $|a_m\rangle |0\rangle^{\otimes n-1}$, where $|a_m\rangle$ takes four states as $|0\rangle$, $|1\rangle$, $|+\rangle$ and $|\rangle + \rangle$. $M_m$ can be obtained using the corresponding measurement results. Refer to Appendix A for the details of the procedure. Also, since $|\phi^m\rangle$ is orthogonal, $A = 1$ and $A_m$ does not have to be calculated.

Finally, we show the procedure to obtain $\langle \psi_{HT} | O | \psi_{HT} \rangle$, which can be implemented by contracting $M_m$ and $A_m$. Now, denoting $|\psi\rangle = \sum_{i_1,i_2,\ldots,i_k} \psi_{i_1,i_2,\ldots,i_k} |i_1 i_2 \ldots i_k\rangle$, we can rewrite Eq. (3) as

$$A^2 \langle O \rangle = \langle \psi | \bigotimes_{m=1}^k M_m | \psi \rangle = \langle \psi | \bigotimes_{m=1}^k U_m^\dagger D_m U_m | \psi \rangle,$$

where we have used the fact that $M_m$ is a Hermitian operator and has a spectral decomposition, $M_m = U_m^\dagger D_m U_m$.

Figure 2(d) shows a quantum circuit to measure $M_m$. Henceforth, we will assume $|\psi\rangle = U_M |0\rangle^{\otimes n}$, where $U_M$ is a unitary operator with polynomial depth. We can compute $A^2 \langle O \rangle$ by applying $U_m$, measuring in a computational basis, and assigning elements of $D_m$ to the measurement results. More concretely, denoting $D_m = \text{diag}[\lambda_{i_m=0}^{(m)}, \lambda_{i_m=1}^{(m)}]$, the measured value is computed as $\prod_{m=1}^k \lambda_{i_m}^{(m)}$ corresponding to the measured outcome $i = (i_1, i_2, \ldots, i_k)$. In a similar procedure, we can measure $A^2$ by contracting $A_m$; hence, we can obtain $\langle O \rangle$.

### III. Calculation of Transition Amplitudes and Overlaps

We describe the measurement of transition amplitudes with the hybrid tensor network approach. The difference
from Sec. II is that we need to contract a non-Hermitian operator $N_m$.

A. Contraction of quantum tensors in subsystems

This section describes construction of $N_m$ in the calculation of $\langle \psi^{(1)}_{HT} | O | \psi^{(2)}_{HT} \rangle$ in the transition amplitudes and that of $\langle \psi^{(1)}_{HT} | \psi^{(2)}_{HT} \rangle$ in the overlaps, where $| \psi^{(1)}_{HT} \rangle$ and $| \psi^{(2)}_{HT} \rangle$ are different states represented by a quantum-quantum tensor network.

To begin with, we will consider the calculation of the transition amplitude because the overlap is a special case of $O = I$ in the transition amplitude, where $I$ is the identity operator. We will comment on the overlap at the end of this section. The transition amplitude $T$ can be defined as

$$T = \frac{1}{A^{(1)}A^{(2)}} \langle \psi^{(1)}_{HT} | O | \psi^{(2)}_{HT} \rangle$$

where

$$T = \frac{1}{A^{(1)}A^{(2)}} \sum \frac{\psi^{(1)}_{i_1} \cdots \psi^{(2)}_{i_k}}{n_{m_k}} \prod_{m=1}^{k} N_{m_k}^{i_{m_k}}$$

and $A^{(l)}$ ($l = 1, 2$) is a normalization constant corresponding to $| \psi^{(l)}_{HT} \rangle$, $i_k = (i_1, i_2, \ldots, i_k)$. $N_m$ is a $2 \times 2$ matrix with elements of $N_m^{i_1i_2} = \langle \phi^{i_1}_{m} | O_m | \phi^{i_2}_{m} \rangle$, and $| \psi^{(l)}_{HT} \rangle = \sum l \psi^{(l)}_{i_l} \cdots \psi^{(l)}_{i_k} | i_1 \cdots i_k \rangle$. The notation is the same as in Eqs. (4), (5) and (6), except for the superscript $(l)$, which corresponds to $| \psi^{(l)}_{HT} \rangle$. The reason that $N_m$ is a non-Hermitian matrix comes from the fact that $(N_m^{i_{m_k}})^* \neq N_m^{i_{m_k}i_{m_k}}$. We will not discuss $A^{(l)}$ in the following since the procedure for calculating $A^{(l)}$ is the same as the one for $A$ in the previous section.

First, let us consider the case of $| \phi^{m}(l) \rangle = U^{m\dagger}(l) | 0 \rangle^{\otimes n}$. Figure 3(a) shows the quantum circuit for constructing $N_m$. The flow of constructing $N_m$ is similar to that of $M_m$. However, since $N_m$ is a $2 \times 2$ non-Hermitian matrix with elements of complex numbers, eight types of measurement are required to construct $N_m$. Next, we consider the case of $| \phi^{m}(l) \rangle = U^{m\dagger}(l) | i_m \rangle | 0 \rangle^{\otimes (n-1)}$. Figure 3(b) shows a quantum circuit to obtain the matrix element $N_{m,m_k}^{i_{m_k}i_{m_k}}$. Specifically, the wave function is initialized by using one of the four types of unitary gates $U_{init}$ in the lower panel in Fig. 3(b) to prepare the initial states $| i_{m_k} \rangle | 0 \rangle^{\otimes (n-1)}$. The subsequent process is the same as in the case of $| \phi^{m}(l) \rangle = U^{m\dagger}(l) | 0 \rangle^{\otimes n}$.

When calculating the overlap $S$, i.e., the case of $O = I$ in Eq. (6), only the circuits to construct $N_m$ (Figs. 3(a) and (b)) differ from the cases of the transition amplitude. Figures 3(c) and (d) shows the circuits in the cases of $| \phi^{m}(l) \rangle = U^{m\dagger}(l) | i_m \rangle | 0 \rangle^{\otimes n-1}$, which are the same quantum circuits as in Figs. 3(a) and (b) except that the measurements of the system qubits are not involved. Note that although the calculation of the transition amplitude and the overlap requires the construction of non-Hermitian operators using the ancilla qubit in general, it can be circumvented in the calculation of the square of the overlap by using the destructive SWAP test [36] (Appendix B for details).

B. Contraction of non-Hermitian matrices

The next step is to calculate $\langle \psi^{(1)} | \bigotimes_{m=1}^{k} N_m | \psi^{(2)} \rangle$ for $2 \times 2$ non-Hermitian matrices $N_m$. We describe two methods: contraction: a Monte-Carlo contraction method and an SVD contraction method. In this section, we describe the SVD contraction method because it is exponentially more efficient than the Monte-Carlo contraction method in terms of the sampling cost. Refer to Appendixes C and D for details of the Monte-Carlo contraction method and the comparison of the two methods, respectively.

Now let us describe how to perform the SVD contraction method. We perform SVD $N_m = B_m^\dagger D_m^\dagger C_m$ for each $N_m$, that is, $\bigotimes_{m=1}^{k} N_m = \bigotimes_{m=1}^{k} B_m^\dagger D_m^\dagger C_m$, where $B_m$ and $C_m$ are unitary matrices and $D_m$ is a diagonal matrix with non-negative elements. $\langle \psi^{(1)} | \bigotimes_{m=1}^{k} N_m | \psi^{(2)} \rangle$ can be described as

$$\langle \psi^{(1)} | \bigotimes_{m=1}^{k} N_m | \psi^{(2)} \rangle = \langle \psi^{(1)} | \bigotimes_{m=1}^{k} B_m^\dagger D_m^\dagger C_m | \psi^{(2)} \rangle$$

where $\langle \psi^{(1)} | \bigotimes_{m=1}^{k} B_m^\dagger D_m^\dagger C_m | \psi^{(2)} \rangle = 2(\prod_{m=1}^{k} \| N_m \|_{op} \cdot \frac{1}{2} \times \text{Re}(\langle \psi^{(1)} | \bigotimes_{m=1}^{k} B_m^\dagger D_m^m C_m | \psi^{(2)} \rangle)) = \text{Im}(\langle \psi^{(1)} | \bigotimes_{m=1}^{k} B_m^\dagger D_m^m C_m | \psi^{(2)} \rangle))$, where $\| A \|_{op}$ is the operator norm of an operator $A$, $d^m(m) = D^m/\| N_m \|_{op}$. We can assume that $d^m(m) = \text{diag}(\lambda^{m}_0, \lambda^{m}_1)$, where $\lambda^{m}_0 \geq \lambda^{m}_1 \geq 0$. $\lambda^{m}_0 = 1$, and $\lambda^{m}_1$ takes a value in a range $[0, 1]$, without loss of generality.

Figure 3(e) shows the circuit for measuring $\langle \psi^{(1)} | \bigotimes_{m=1}^{k} N_m | \psi^{(2)} \rangle$ by using the SVD contraction method. We can compute $\langle \psi^{(1)} | \bigotimes_{m=1}^{k} N_m | \psi^{(2)} \rangle$ as follows. We implement a Hadamard test circuit for $\bigotimes_{m=1}^{k} B_m^\dagger D_m^m C_m$ for obtaining the real or imaginary part of $\langle \psi^{(1)} | \bigotimes_{m=1}^{k} N_m | \psi^{(2)} \rangle$ with probability 1/2 (i.e., 1:1 ratio) by changing the phase of the ancilla qubit.
FIG. 3. Quantum circuits for obtaining transition amplitudes and overlaps. In all the figures, the topmost line represents an ancilla qubit and the other lines represent system qubits. Real and imaginary components are obtained by setting \( \alpha = 0 \) and \( \alpha = \frac{\pi}{2} \), respectively. A white (black) circle in a controlled gate means that a unitary operation is performed on the target qubits when the control qubit is \( |0\rangle \) (\( |1\rangle \)).

(a) A quantum circuit to construct \( N_m \) for calculating transition amplitudes in the case of \( |\phi_m^{(l)}\rangle = U_{Cm}^{(l)} |0\rangle \otimes n \). (b) A quantum circuit to construct \( N_m \) for calculating transition amplitudes in the case of \( |\phi_m^{(l)}\rangle = U_{Cm}^{(l)} i_m |0\rangle \). (c) A quantum circuit to construct \( N_m \) for calculating overlaps in the case of \( |\phi_m^{(l)}\rangle = U_{Cm}^{(l)} |0\rangle \otimes n \). (d) A quantum circuit to construct \( N_m \) for calculating overlaps in the case of \( |\phi_m^{(l)}\rangle = U_{Cm}^{(l)} i_m |0\rangle \). (e) A quantum circuit to measure \( N_m \) for calculating transition amplitudes or overlaps.

We define \( \mu_s^{(Re)} = 2(\prod_{m=1}^{k} \|N_m\|_{op})(\prod_{m=1}^{k} \tilde{\lambda}_{m,s}^{(m)}) b_s \) and \( \mu_s^{(Im)} = 2i(\prod_{m=1}^{k} \|N_m\|_{op})(\prod_{m=1}^{k} \tilde{\lambda}_{m,s}^{(m)}) b_s \) in the cases of measurements of the real and imaginary parts, respectively, where \( i_m \in \{0, 1\} \) and \( b_s \in \{-1, 1\} \) are the measurement outcomes of the system and ancilla qubits in the \( s \)-th measurement, respectively. Then, the sum of the total sample averages of each of \( \mu_s^{(Re)} \) and \( \mu_s^{(Im)} \) approximates \( \langle \psi^{(1)} | \otimes_{m=1}^{k} N_m |\psi^{(2)}\rangle \).

Letting \( \bar{x} \) denote the sample average of a random variable \( x \), \( E[x] \) denotes the expected value of \( x \), and \( \bar{\mu}_s = \mu_s^{(Re)} + \mu_s^{(Im)} \) approximates \( \langle \psi^{(1)} | \otimes_{m=1}^{k} N_m |\psi^{(2)}\rangle \). Denoting the number of measurements as \( N_{SV D} \) and assuming \( \forall m \|N_m\|_{op} = \|N_{const}\|_{op} \), we have

\[
E[|\bar{\mu}_s - \langle \psi^{(1)} | \otimes_{m=1}^{k} N_m |\psi^{(2)}\rangle|] = O\left(\frac{\|N_{const}\|_{op}^k}{\sqrt{N_{SV D}}}\right).
\]

(8)

Thus, we have

\[
N_{SV D} = O\left(\frac{\|N_{const}\|_{op}^{2k}}{\varepsilon^2}\right)
\]

(9)

for the required accuracy \( \varepsilon \).

We mention that \( N_{SV D} \) is expected not to increase exponentially with \( k \) if \( n \) is large enough. Here, we consider
the case where the measured observable \( O \) is a product of Pauli operators. This is because in the conventional variational quantum eigensolver (VQE) \([13]\) scenario, we decompose the Hermitian operator of interest into a linear combination of a polynomial number of products of Pauli operators with the system size. We numerically generate four types of \( 2^n \times 2^n \) random unitary matrices, \( U^{(0)}(1), U^{(1)(1)}, U^{(2)(2)}, \) and \( U^{(3)(3)} \), and a product of random Pauli operators, \( O_{\text{rand}} \), and create a \( 2 \times 2 \) matrix \( N_{\text{const}} \) consisting of elements \( N_{\text{const}} = \langle 0 \| U^{(1)}(1)O_{\text{rand}}U^{(2)(2)} \| 0 \rangle \otimes n = \langle i \| \), where \( i \) and \( j \) take 0 or 1. Then, we evaluate the average values of \( \| N_{\text{const}} \|_{op} \) obtained using 10,000 samples of \( N_{\text{const}} \). As a result, we obtain \( \| N_{\text{const}} \|_{op} < 1 \), including error bars when \( n \geq 3 \) (See Appendix \( D \) for details). Therefore, if \( n \) is large enough, \( N_{\text{SV}} \leq O(1/\varepsilon^2) \) will be valid.

Additionally, we should note that in the case of \( \langle \varphi^{\text{in}}(i) \| = U^{(1)}(i) | i \rangle | 0 \rangle \otimes n-1 \), \( N_{\text{SV}} \leq O(1/\varepsilon^2) \) is strictly satisfied regardless of \( n \). In this case, since \( N_{m} \) can be regarded as a submatrix of the unitary matrix \( U^{(1)(2)} \), \( \| N_{m} \|_{op} \leq \| O_{m} \|_{op} \). Thus, because we have assumed \( \| O_{m} \|_{op} = 1 \), we have \( N_{\text{SV}} \leq O(1/\varepsilon^2) \) regardless of \( n \).

IV. CONCLUSION

We proposed a method to calculate transition amplitudes using a hybrid tensor network. When the hybrid tensor network approach is naively applied to the transition amplitude calculation, the contracted operators become non-Hermitian, and the number of terms to be measured increases exponentially. Our method obtains the expectation value without increasing the number of terms exponentially by using singular value decomposition and a Hadamard test. Our theory can be easily generalized to cases with a mixture of classical and quantum tensors called quantum-classical and classical-quantum tree-tensor networks, and those with deeper tree structures. Moreover, we can easily extend the scenario to the case where the measured operator \( O \) is a tensor product of non-Hermitian operators by using the SVD contraction method. This study significantly expands the applicability of the hybrid tensor network.

Future work includes the application of our method to algorithms related to hybrid tensor networks. For example, Deep VQE, \([20, 21]\), which is a large-scale computational algorithm for NISQ devices based on the divide and conquer method, can be treated in the framework of hybrid tensor networks in theory. By applying the proposed method to such algorithms, we can extend the range of applications to various large-scale quantum algorithms.

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Appendix A: Construction of $M_m$ in the case where indices $i_n$ are mapped to initial wave functions

We explain the procedure of constructing $M_m$ in the case of $|\phi_i\rangle = U_C m |i_m\rangle |0\rangle^\otimes n-1$ by using the circuit in Fig. 2(c). The diagonal elements, $M_{0m}$ and $M_{11}$, can be easily obtained by measuring the expectation values of $O_m$ for $|\phi_i\rangle^0$ and $|\phi_i\rangle^1$ because $M_{0m} = \langle \phi_i^0 | O_m | \phi_i^0 \rangle$ and $M_{11} = \langle \phi_i^1 | O_m | \phi_i^1 \rangle$, respectively. We can also obtain non-diagonal elements by combining four types of measurement results. By setting $\langle + | m \rangle = (|\phi_i^0\rangle + |\phi_i^1\rangle)/\sqrt{2}$ and $\langle + | y | m \rangle = (|\phi_i^0\rangle + i |\phi_i^1\rangle)/\sqrt{2}$, we have

$$\langle + | m \rangle | O_m \rangle | + | m \rangle = \frac{1}{2} (M_{00} + M_{01} + M_{10} + M_{11})$$

and

$$\langle + | y | m \rangle | O_m \rangle | + | y | m \rangle = \frac{1}{2} (M_{00} + i M_{01} - i M_{10} + M_{11}).$$

Then, we can obtain the non-diagonal elements by

$$M_{01} = \frac{i - 1}{2} \langle \phi_i^{0m=0} | O_m | \phi_i^{0m=0} \rangle$$

$$+ \frac{i - 1}{2} \langle \phi_i^{1m=1} | O_m | \phi_i^{1m=1} \rangle$$

$$+ \langle + | m \rangle | O_m \rangle | + | m \rangle$$

$$- i \langle + | y | m \rangle | O_m \rangle | + | y | m \rangle$$

and $M_{10} = M_{01}^*$. 

Appendix B: Calculation of the square of overlaps without the ancilla qubit

In this section, we show the procedure of the calculation for the square of overlaps $| \langle \psi_{HT}^{(1)} | \psi_{HT}^{(2)} \rangle |^2$ by using the destructive SWAP test without using the ancilla qubit. The main point of the procedure is that we regard $| \langle \psi_{HT}^{(1)} | \psi_{HT}^{(2)} \rangle |^2$ as the expectation value of the SWAP operator for the 2nk state $| \tilde{\psi}_{HT} \rangle = | \psi_{HT}^{(1)} \rangle | \psi_{HT}^{(2)} \rangle$, where
$|\psi_{1n}'\rangle$ and $|\psi_{2n}'\rangle$ are two different states represented by a quantum-quantum tensor network. Since the SWAP operator is an observable, we can calculate $|\langle \psi_{1n}'|\psi_{2n}'\rangle|^2$ by following almost the same procedure as Sec. [3] without the ancilla qubit.

Specifically, letting the SWAP operator $SWAP = \bigotimes_{k}^{m-1} SWAP_{m}$ and $SWAP_{m} = \bigotimes_{r=1}^{n} SWAP_{mr}$ and substituting $|\psi_{1n}'\rangle$ for $|\psi_{1n}\rangle$ and SWAP for $O$ in Eq. [3], the square of overlaps $|\langle \psi_{1n}'|\psi_{2n}'\rangle|^2$ can be obtained from the expectation value $\langle SWAP \rangle$ as

$$\langle SWAP \rangle = \langle \tilde{\psi}_{1n}|SWAP|\tilde{\psi}_{1n}\rangle$$

$$= \langle \psi_{1n}'|\langle \psi_{2n}'|SWAP|\psi_{1n}'\rangle|\psi_{2n}'\rangle$$

$$= \langle \langle \psi_{1n}'\rangle \langle \psi_{2n}'\rangle | \bigotimes_{m=1}^{k} M_{m}^{\dagger}|\psi_{1n}\rangle|\psi_{2n}\rangle,$$

and $\langle SWAP \rangle$ can be also described as

$$\langle SWAP \rangle = \sum_{\tilde{i}_{(1)}^{(2)}, m} \psi_{\tilde{i}_{(1)}^{(2)}}^{(1)} \psi_{\tilde{i}_{(2)}^{(2)}}^{(1)} \psi_{\tilde{i}_{(1)}^{(2)}}^{(2)} \psi_{\tilde{i}_{(2)}^{(2)}}^{(2)} \prod_{m=1}^{k} M_{m}^{\dagger} m|\tilde{i}_{(1)}^{(2)} m|\tilde{i}_{(2)}^{(2)} m\rangle,$$

where $\tilde{i}_{(l)} = (i_{(1)}, i_{(2)}, \ldots, i_{(l)})$ $(l = 1, 2)$ with $i_{(m)}$ taking either 0 or 1, and $M_{m}$ is a $4 \times 4$ matrix with elements of

$$M_{m}^{\dagger}(1)m|\tilde{i}_{(1)}^{(2)} m|\tilde{i}_{(2)}^{(2)} m\rangle = \langle \varphi_{(1)}^{(1)}|\langle \varphi_{(2)}^{(2)}|SWAP_{mr}|\varphi_{(1)}^{(1)}\rangle|\varphi_{(2)}^{(2)}\rangle$$

$= \langle \varphi_{(1)}^{(1)}|\langle \varphi_{(2)}^{(2)}|SWAP_{mr}|\varphi_{(1)}^{(1)}\rangle|\varphi_{(2)}^{(2)}\rangle.$

Here, $M_{m}$ is an observable on $m$-th qubits of $|\psi_{1n}'\rangle$ and $|\psi_{2n}'\rangle$, and $SWAP_{mr}$ is an observable on $r$-th qubits of $|\varphi_{(1)}^{(1)}\rangle$ and $|\varphi_{(2)}^{(2)}\rangle$. We consider only the case of $|\varphi_{(1)}^{(1)}\rangle = U_{m}^{(1)}|\tilde{i}_{(m)}\rangle |0\rangle^{\otimes n-1}$, and thus we omit the normalization constant.

Figure 4(a) shows a quantum circuit to obtain the matrix element $M_{m}^{\dagger}|\tilde{i}_{(1)}^{(2)} m|\tilde{i}_{(2)}^{(2)} m\rangle$ using the destructive SWAP test. The procedure of obtaining the matrix elements is as follows. Firstly, the initial states are set to $|a_{(1)m}\rangle |0\rangle^{\otimes n-1}$ $|a_{(2)m}\rangle |0\rangle^{\otimes n-1}$, where $|a_{(l)m}\rangle$ takes four states as $|0\rangle$, $|1\rangle$, $|+\rangle$ and $|+\rangle$. To construct $M_{m}$, $4 \times 16$ types of the states are required in total (Table 1). After preparing the states $(U_{Cm}^{(1)} \otimes U_{Cm}^{(2)} |a_{(1)m}\rangle |0\rangle^{\otimes n-1} |a_{(2)m}\rangle |0\rangle^{\otimes n-1}$, unitary gates for the measurement $\tilde{U}_{mr}$ consisting of CNOT gates and Hadamard gates $H$ are applied. Here, $\tilde{U}_{mr}$ is obtained by the spectral decomposition of $SWAP_{mr}$ as $SWAP_{mr} = U_{mr}^{(1)} D_{mr} U_{mr}^{(2)}$, where $U_{mr}$ is a unitary matrix and $D_{mr}$ is a diagonal matrix. Finally, we assign elements of $D_{mr}^{\dagger}$ to the measurement results from each qubit pair.

Figure 4(b) shows a quantum circuit to construct $M_{m}$. We can obtain $|\langle \psi_{1n}'\rangle|\langle \psi_{2n}'|\bigotimes_{m=1}^{k} M_{m}^{\dagger}|\psi_{1n}'\rangle|\psi_{2n}'\rangle$ by preparing $|\psi_{1n}'\rangle|\psi_{2n}'\rangle = (U_{m}^{(1)} \otimes U_{m}^{(2)} |0\rangle^{\otimes k} |0\rangle^{\otimes k}$, applying unitary gates for the measurement $\tilde{U}_{m}$, and assigning elements of $D_{m}$ to the measurement results from each qubit pair, where $M_{m}^{\dagger} = \tilde{U}_{m}^{\dagger} D_{m} U_{m}^{(1)}$, $\tilde{U}_{m}$ is a unitary matrix, and $D_{m}$ is a diagonal matrix.

Since the destructive SWAP test circumvents the use of ancilla qubits and the effects of additional noise, it should be used in algorithms such as the variational quantum deflation for evaluating excited states [38] and variational quantum state diagonalization [39].
Appendix C: Monte-Carlo contraction method

In this section, we introduce a Monte-Carlo contraction method and discuss the sampling cost. We decompose \( \bigotimes_{m=1}^{k} N_m = \bigotimes_{m=1}^{k} (h_{1m} I_m + h_{Xm} X_m + h_{Ym} Y_m + h_{Zm} Z_m) \), where \( I_m \) is an identity operator, \( X_m, Y_m \) and \( Z_m \) are Pauli operators which act on the \( m \)-th qubit, and \( h_{\alpha} (\alpha \in \{ I_m, X_m, Y_m, Z_m \}) \) are the corresponding coefficients. If we expand the last expression, it has an exponentially increasing number of terms with \( k \). To circumvent this problem, a Monte-Carlo implementation can be used to calculate \( \langle \psi^{(1)} | \bigotimes_{m=1}^{k} N_m | \psi^{(2)} \rangle \). From now on, for notational simplicity, we will denote \( \sigma_{0}^{(m)} = I_m \), \( \sigma_{1}^{(m)} = X_m \), \( \sigma_{2}^{(m)} = Y_m \), \( \sigma_{3}^{(m)} = Z_m \), \( h_{0}^{(m)} = h_{1m} \), \( h_{1}^{(m)} = h_{Xm} \), \( h_{2}^{(m)} = h_{Ym} \), and \( h_{3}^{(m)} = h_{Zm} \). Introducing \( \gamma^{(m)} = \sum_{k=0}^{3} | h_{k}^{(m)} |, p_{k}^{(m)} = | h_{k}^{(m)} | / \gamma^{(m)} \), \( \phi_{i}^{(m)} \in \mathbb{R} \), and \( e^{i \phi_{i}^{(m)}} = h_{i}^{(m)} / h_{i}^{(m)} \), we have \( \sum_{i} p_{i}^{(m)} = 1 \) and

\[
\langle \psi^{(1)} | \bigotimes_{m=1}^{k} N_m | \psi^{(2)} \rangle = 2 \left( \prod_{m=1}^{k} \gamma^{(m)} \right) \sum_{i_{1}, i_{2}, \ldots, i_{k}} \left( \prod_{m=1}^{k} p_{i_{m}}^{(m)} \right) \cdot \frac{1}{2} \times e^{i \sum_{m=1}^{k} \phi_{i_{m}}} \times [\text{Re}(\langle \psi^{(1)} | \bigotimes_{m=1}^{k} \sigma_{i_{m}}^{(m)} | \psi^{(2)} \rangle) + i \text{Im}(\langle \psi^{(1)} | \bigotimes_{m=1}^{k} \sigma_{i_{m}}^{(m)} | \psi^{(2)} \rangle)].
\]

(C1)

Therefore, we can compute \( \langle \psi^{(1)} | \bigotimes_{m=1}^{k} N_m | \psi^{(2)} \rangle \) as follows. We generate \( \bigotimes_{m=1}^{k} \sigma_{i_{m}}^{(m)} \) with probability \( \prod_{m=1}^{k} p_{i_{m}}^{(m)} \) and implement a Hadamard test circuit for obtaining the real or imaginary part of \( \langle \psi^{(1)} | \bigotimes_{m=1}^{k} N_m | \psi^{(2)} \rangle \) with probability 1/2 (i.e., 1:1 ratio) by changing the phase of the ancilla qubit. We define \( \mu_{s}^{(\text{Re})} = 2(\prod_{m=1}^{k} \gamma^{(m)} \gamma) \sum_{i_{1}, i_{2}, \ldots, i_{k}} \phi_{i_{m}}^{(m)} b_{s}^{(m)} \) and \( \mu_{s}^{(\text{Im})} = 2(\prod_{m=1}^{k} \gamma^{(m)} \gamma) \sum_{i_{1}, i_{2}, \ldots, i_{k}} \phi_{i_{m}}^{(m)} b_{s}^{(m)} \) in the cases of measurements of the real and imaginary parts, respectively, where \( b_{s}^{(m)} \in \{-1, 1\} \) is the measurement outcomes of the ancilla qubit in the \( s \)-th measurement. Then, the sum of the total sample averages of each of \( \mu_{s}^{(\text{Re})} \) and \( \mu_{s}^{(\text{Im})} \) approximates \( \langle \psi^{(1)} | \bigotimes_{m=1}^{k} N_m | \psi^{(2)} \rangle \).

Below, \( \bar{x} \) denotes the sample average of a random variable \( x \), \( E[x] \) denotes the expected value of \( x \), and \( \bar{\mu}_{s}^{(\text{Re})} = \mu_{s}^{(\text{Re})} + \mu_{s}^{(\text{Im})} \) approximates \( \langle \psi^{(1)} | \bigotimes_{m=1}^{k} N_m | \psi^{(2)} \rangle \). Denoting the number of measurements as \( N_{MC} \) and assuming \( \forall m \gamma^{(m)} = \gamma \), we have

\[
E[\bar{\mu}_{s}^{(\text{Re})} - \langle \psi^{(1)} | \bigotimes_{m=1}^{k} N_m | \psi^{(2)} \rangle] = O(\gamma^{k} / \sqrt{N_{MC}}).
\]

(C2)

Thus, we need

\[
N_{MC} = O(\gamma^{2k} / \varepsilon^{2})
\]

(C3)

for the required accuracy \( \varepsilon \).
Appendix D: Comparison of Monte-Carlo contraction method and SVD contraction method

Here, we compare $N_{MC}$ with $N_{SVD}$. Since $N_m = \sum_i h_{im} \sigma_i^{(m)}$, we have

$$\|N_m\|_{op} \leq \sum_i |h_{im}| \|\sigma_i^{(m)}\|_{op} = \gamma^{(m)},$$  \hspace{1cm} (D1)

where we have used $\|\sigma_i^{(m)}\|_{op} = 1$.

Equations (9), (C3), and (D1) indicate $\gamma/\|N_{const}\|_{op} \geq 1$ and

$$\frac{N_{MC}}{N_{SVD}} = O((\gamma/\|N_{const}\|_{op})^{2k}).$$  \hspace{1cm} (D2)

Thus, the SVD contraction method is exponentially more efficient than the Monte-Carlo contraction method in terms of the sampling cost.

We present numerical calculations for $\gamma/\|N_{const}\|_{op}$ in order to check the superiority of the SVD contraction method over the Monte-Carlo contraction method. We obtain 10,000 samples of $N_{const}$ and $\|N_{const}\|_{op}$ by the procedure in Sec. III B and $\gamma$ from the Pauli decomposition of $N_{const}$. Fig. 5(a) shows the average of the ratio $\gamma/\|N_{const}\|_{op}$; we found that the average value is about 1.4 for any $n$. Therefore, from Eq. (D2) and the result in Fig. 5(a), we can conclude that the SVD contraction method is expected to be $O((1.4)^{2k})$ times faster on average than the Monte-Carlo contraction method.

We also numerically evaluate the number of measurements for the two methods. The averages of $\gamma$ and $\|N_{const}\|_{op}$ are shown in Fig. 5(b). $\gamma$ and $\|N_{const}\|_{op}$ in $n \geq 4$ and $n \geq 3$, respectively, can be considered to be less than 1, including the standard deviation. Thus, we expect $N_{MC} \leq O(1/\varepsilon^2)$ and $N_{SVD} \leq O(1/\varepsilon^2)$; that is, $N_{MC}$ and $N_{SVD}$ are not expected to increase exponentially with $k$, if $n$ is large enough.

FIG. 5. Average values of $\gamma/\|N_{const}\|_{op}$, $\gamma$, and $\|N_{const}\|_{op}$ depending on the number of qubits $n$ (10,000 samples). Each point and error bar represent the average value and standard deviation of the samples, respectively. (a) Average value of $\gamma/\|N_{const}\|_{op}$. (b) Average values of $\gamma$ (circled, red) and $\|N_{const}\|_{op}$ (diamond, blue).