Macroscopic Entanglement in Quantum Computation

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We investigate macroscopic entanglement of quantum states in quantum computers, where we say a quantum state is entangled macroscopically if the state has superposition of macroscopically distinct states. The index $p$ of the macroscopic entanglement is calculated as a function of the step of the computation, for Grover’s quantum search algorithm and Shor’s factoring algorithm. It is found that whether macroscopically entangled states are used or not depends on the numbers and properties of the solutions to the problem to be solved. When the solutions are such that the problem becomes hard in the sense that classical algorithms take more than polynomial steps to find a solution, macroscopically entangled states are always used in Grover’s algorithm and almost always used in Shor’s algorithm. Since they are representative algorithms for unstructured and structured problems, respectively, our results support strongly the conjecture that quantum computers utilize macroscopically entangled states when they solve hard problems much faster than any classical algorithms.

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I. INTRODUCTION

Quantum computers are many-body systems with a large but finite number $L$ of qubits because the efficiency of computation becomes relevant only when $L$ is large $\frac{1}{2}$. Although the entanglement is considered to play crucial roles in speedup as compared with classical computers $\frac{2}{2}$, there are many types of entanglement and many measures or indices of entanglement for many-body systems $\frac{3}{3}$, $\frac{4}{4}$, $\frac{5}{5}$, $\frac{6}{6}$, $\frac{7}{7}$, $\frac{8}{8}$, $\frac{9}{9}$, $\frac{10}{10}$, $\frac{11}{11}$, $\frac{12}{12}$, $\frac{13}{13}$. It is therefore interesting to explore which type of entanglement is relevant and which measure or index quantifies such entanglement.

Recently, an index $p$ of macroscopic entanglement, which implies that the state has superposition of macroscopically distinct states, was proposed and studied in Refs. $\frac{11}{11}$, $\frac{12}{12}$, $\frac{13}{13}$: A pure state, which is homogeneous or effectively homogeneous (see Refs. $\frac{4}{4}$, $\frac{11}{11}$, $\frac{13}{13}$ and Secs. $\frac{IV}{IV}$-$\frac{VI}{VI}$), is entangled macroscopically iff it has $p = 2$. Although the term ‘macroscopic entanglement’ are sometimes used in different ways, we follow these references. Most importantly, the macroscopic entanglement as defined by this index is directly related to fundamental stabilities of many-body quantum states (see Ref. $\frac{11}{11}$ and Sec. $\frac{II}{II}$). Moreover, it was shown rigorously that any pure states with $p = 2$ in systems of finite $L$ do not approach pure states in the infinite system as $L \rightarrow \infty$ $\frac{11}{11}$, $\frac{14}{14}$. Noting that macroscopically entangled states have such anomalous properties, one of the authors gave the conjecture that a quantum computer should utilize macroscopically entangled states in some stages of the computation when it performs a quantum algorithm that is much more efficient than any classical algorithms (Ref. $\frac{15}{15}$ and Sec. $\frac{III}{III}$).

In the previous paper $\frac{11}{11}$, we confirmed this conjecture in the case of Shor’s factoring algorithm $\frac{14}{14}$, $\frac{15}{15}$. Since Shor’s algorithm is a representative quantum algorithm for solving structured problems $\frac{1}{1}$, it is very interesting to study whether the conjecture is correct in the case of quantum algorithms for solving unstructured problems $\frac{1}{1}$. Furthermore, in Ref. $\frac{11}{11}$ we identified macroscopic entanglement of only two states, the state after the modular exponentiation and the final state, among many quantum states appearing in Shor’s algorithm, because it was difficult to identify macroscopic entanglement of general states. It is also interesting to study whether the other states in Shor’s algorithm are entangled macroscopically. Recently, an efficient method of calculating the index $p$ was developed and successfully applied to many-magnon states $\frac{12}{12}$ and to chaotic many-body states $\frac{13}{13}$. This method, called the variance-covariance matrix (VCM) method, enables us to study the macroscopic entanglement of general states.

In this paper, we study macroscopic entanglement of quantum states of quantum computers performing Grover’s quantum search algorithm $\frac{13}{13}$, which is a representative algorithm for solving unstructured problems $\frac{1}{1}$. The results show that the above conjecture is correct also in this case. We also investigate macroscopic entanglement of all quantum states appearing in Shor’s factoring algorithm, using the VCM method, and the above conjecture is confirmed again. These results suggest the relevance of macroscopic entanglement in solving hard problems by quantum computers.

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The paper is organized as follows. In Sec. II, we briefly explain the index \( p \) of the macroscopic entanglement. Section III restates the conjecture in a more detailed form than Refs. [4] and [15]. Analytic results for Grover’s quantum search algorithm are given in Sec. IV, by which the conjecture is confirmed. To see details of evolution of entanglement, we present results of numerical simulations of a quantum computer that performs Grover’s quantum search algorithm in Sec. V. Shor’s factoring algorithm is studied in Sec. VI, and the conjecture is again confirmed. Discussions and conclusions are given in Sec. VII.

II. INDEX OF MACROSCOPIC ENTANGLEMENT

The index \( p \) of macroscopic entanglement was proposed and studied in Refs. [11, 12, 13]. In this section, we briefly explain it to establish the notations and for reader’s convenience.

A. Definition

We consider quantum states which are homogeneous, or effectively homogeneous as in quantum chaotic systems [13] and in quantum computers (see Secs. IV, VII, and Ref. [4]). For such a state, we consider a family of similar states of various sizes, and denote the state of size \( L \) of \( \psi \). We say \( \rho(L) \) (or a quantum system) is macroscopic if for every quantity of interest the term that is leading order in \( L \) gives the dominant contribution [19]. We say \( \rho(L) \) is entangled macroscopically if the state has ‘superposition of macroscopically distinct states’ [11, 12, 19, 20].

In general, however, the term in the quotation marks is quite ambiguous [12, 19]. For example, it would be obvious that a ‘cat state’ \( |\psi_{\text{cat}}(L)\rangle = (|00\cdots0\rangle + |11\cdots1\rangle)/\sqrt{2} \) of a quantum computer with \( L \) qubits has such superposition, whereas how about the following state [12]?

\[
|\psi_{\text{dws}}(L)\rangle \equiv \frac{1}{\sqrt{L+1}}(|00\cdots0\rangle + |100\cdots0\rangle + |110\cdots0\rangle + \cdots + |111\cdots1\rangle). \tag{1}
\]

Recently, a reasonable index \( p \) of macroscopic entanglement was proposed for pure states [11, 12] For \( \hat{\rho}(L) = |\psi(L)\rangle\langle\psi(L)| \), this index is defined by [21]

\[
\max_{\hat{A}} \langle \psi(L) | \Delta \hat{A} \Delta | \psi(L) \rangle = O(L^p), \tag{2}
\]

where \( \Delta \hat{A} \equiv \hat{A} - \langle \psi(L) | \hat{A} | \psi(L) \rangle \) and \( \hat{A} \) is an additive operator, i.e., a sum of local operators [11]; see, e.g., Eqs. (3) below.

The index \( p \) ranges over \( 1 \leq p \leq 2 \) (see Appendix). According to Refs. [11, 12], a pure state is entangled macroscopically if \( p = 2 \) [20], whereas it may be entangled but not macroscopically if \( p < 2 \). For example, the ‘W state,’ \( |\psi_{\text{W}}(L)\rangle \equiv \frac{1}{\sqrt{L}}(|100\cdots0\rangle + |010\cdots0\rangle + \cdots + |000\cdots1\rangle) \), has \( p = 1 \), hence its entanglement is not macroscopic [11, 12]. This is reasonable because the W state corresponds to a single-magnon state in a ferromagnet, which is quite a normal state. Since both the W state and product states have \( p = 1 \), they belong to the same class with respect to the macroscopic entanglement. On the other hand, we can show that \( p = 2 \) for \( |\psi_{\text{dws}}\rangle \) of Eq. (1), hence is entangled macroscopically. Physically, \( |\psi_{\text{dws}}\rangle \) is superposition of single-domain-wall states which have different positions of the domain wall.

It is worth mentioning that a generalized index \( q \), which can be applied to mixed states as well, and a method for detecting macroscopic entanglement were proposed in Ref. [10]. However, we do not discuss these points in this paper because we treat pure states only.

B. Efficient method of calculating \( p \)

Evaluation of a measure or index of entanglement often becomes intractable for large \( L \). Fortunately, this is not the case for \( p \), i.e., there is an efficient method of calculating \( p [12, 13] \).

For qubit systems, an additive operator can be expressed as

\[
\hat{A} = \sum_{l=1}^{L} \left[ c_{I_0} \hat{I}(l) + \sum_{\alpha=x,y,z} c_{I_0} \hat{\sigma}_\alpha(l) \right]. \tag{3}
\]
Here, \( \hat{1}(l) \) and \( \hat{\sigma}_\alpha(l) \) \((\alpha = x, y, z)\) denote the identity and the Pauli operators, respectively, acting on the qubit at site \( l \), and \( c_{l0}'s \) and \( c_{l0}'s \) are complex numbers which are independent of \( L \). For convenience, we here allow non-hermitian additive operators, as in Refs. [11, 12]. Since we are interested in \( \Delta \hat{A} \), we henceforth drop \( \sum_l c_{l0} \hat{1}(l) \) from Eq. [4 12], i.e.,

\[
\Delta \hat{A} = \sum_{l=1}^{L} \sum_{\alpha=x,y,z} c_{l\alpha} \hat{\sigma}_\alpha(l).
\]

Without loss of generality, we normalize \( c_{l\alpha}'s \) as

\[
\sum_{l=1}^{L} \sum_{\alpha=x,y,z} |c_{l\alpha}|^2 = L.
\]

The \( \max_{\hat{A}} \) in Eq. [2] is thus taken over all possible choices of \( c_{l\alpha}'s \) satisfying this condition.

Let us define the variance-covariance matrix (VCM) for a pure state \( |\psi(L)\rangle \) by

\[
V_{\alpha\beta\prime\prime} = \langle \psi(L)|\Delta \hat{\sigma}_\alpha(l)\Delta \hat{\sigma}_\beta(l')|\psi(L)\rangle,
\]

where \( \Delta \hat{\sigma}_\alpha(l) = \hat{\sigma}_\alpha(l) - \langle \psi(L)|\hat{\sigma}_\alpha(l)|\psi(L)\rangle \), \( \alpha, \beta = x, y, z \), and \( l, l' = 1, 2, \cdots, L \). It was shown in Ref. [12] that the maximum eigenvalue \( e_{\max}(L) \) of the VCM is related to \( p \) of \( |\psi(L)\rangle \) as

\[
e_{\max}(L) = \mathcal{O}(L^{p-1}).
\]

Hence, we can calculate \( p \) by calculating \( e_{\max}(L) \), which can be done in a Poly\((L)\) time because the VCM is a \( 3L \times 3L \) hermitian matrix. Furthermore, from the eigenvector(s) of the VCM corresponding to \( e_{\max}(L) \), we can find the \( \text{maximally-fluctuating additive operator(s)} \ \hat{A}_{\text{max}} \), which satisfies [12, 25]

\[
\max_A \langle \psi(L)|\Delta \hat{A}^{\dagger} \Delta \hat{A}|\psi(L)\rangle = \langle \psi(L)|\Delta \hat{A}_{\text{max}}^{\dagger} \Delta \hat{A}_{\text{max}}|\psi(L)\rangle \sim e_{\max}(L)L = \mathcal{O}(L^p).
\]

C. Physical properties of \( p \)

It was shown in Ref. [11] that \( p \) is directly related to fundamental stabilities, including decoherence and stability against local measurements, of many-body states [22]. Regarding decoherence by weak perturbations from noises or environments, it was shown that for any state with \( p = 1 \) its decoherence rate \( \Gamma \) by any of such perturbations never exceeds \( \mathcal{O}(L) \). For a state with \( p = 2 \), on the other hand, it is possible to theoretically construct a noise or environment that makes \( \Gamma \) of the state \( \mathcal{O}(L^2) \). This does not necessarily mean that such a fatal noise or environment exists in real systems: It depends on physical situations [11]. In this view, a more fundamental stability is the stability against local measurements, which was proposed and defined in Ref. [11]. From the theorem proved there, we can see that a state with \( p = 2 \) is not stable against local measurements, i.e., there exists a local observable by measurement of which the state changes drastically. Furthermore, it was also proved rigorously that any pure states with \( p = 2 \) in systems of finite \( L \) do not approach pure states in the infinite system as \( L \rightarrow \infty [11, 12] \).

These observations indicate that pure states with \( p = 2 \) are quite anomalous many-body states. This led to the conjecture of Ref. [11], which will be restated more clearly in Sec.III. If this conjecture is correct, \( p \) is one of indices that are most directly related to efficiency of quantum computation, among many measures and indices of entanglement. This conjecture has been confirmed in Ref. [4] for Shor’s factoring algorithm, which is a representative algorithm for structured problems, and will be confirmed in this work for Grover’s quantum search algorithm, which is a representative algorithm for unstructured problems.

The index \( p \) was also studied for many-magnon states in Ref. [12], and for many-body chaotic states in Ref. [13]. Comparison with another measure of entanglement were also made in these references. Most importantly, many states were found such that they are almost maximally entangled in another measure but their \( p \) is minimum, \( p = 1 \). Many other states are also found such that their \( p \) is maximum, \( p = 2 \), but their entanglement is small in another measure. This demonstrates the well-known fact that a simple statement such as ‘more efficiency of computation requires more entanglement’ is meaningless unless the measure or index of the entanglement is specified. In this paper, we focus on the macroscopic entanglement as measured by the index \( p \).
III. CONJECTURE ON QUANTUM COMPUTATION

Consider a computational problem, the fastest classical algorithm for which takes $Q^{\text{cl}}_{\text{min}}(L)$ steps when the size of the input is $L$ bits. We consider quantum computers that solves the same problem. Here, to be definite, we mean quantum circuits by ‘quantum computers.’ There are many different circuits for a single quantum algorithm. We say a quantum algorithm $\mathcal{A}$ solves this problem much faster than classical algorithms if some quantum circuit of $\mathcal{A}$ takes only $Q(L)$ steps which is much less than $Q^{\text{cl}}_{\text{min}}(L)$ in the sense that

$$\frac{\ln \left[ \ln Q^{\text{min}}_{\text{cl}}(L) - \ln Q(L) \right]}{\ln L} \geq \text{a positive constant, for large } L.$$  

(9)

Here, in the case of the search problem of Grover, we count each oracle call as one step in defining $Q^{\text{min}}_{\text{cl}}(L)$ and $Q(L)$. Let $\mathcal{L}_0(L)$ be the minimum number of qubits of such circuits that satisfy this inequality. Our conjecture is as follows: If a quantum computer which has $\mathcal{L}(L)$ qubits performs $\mathcal{A}$ with $Q(L)$ steps that satisfies inequality (9), and if

$$\mathcal{L}(L) = \mathcal{L}_0(L) + O(1),$$

(10)

where $O(1)$ denotes a constant that is independent of $L$, then a macroscopically entangled state(s) of size $\mathcal{O}(L)$ or more appears in the quantum computer during the computation [21]. Although it would be hard to determine $\mathcal{L}_0(L)$ of a general algorithm, we assume optimistically in this paper that the simple circuits of Secs. V and VI for Grover’s quantum search and Shor’s factoring algorithms, respectively, would satisfy Eq. (10).

In the case of Grover’s quantum search algorithm, for example, the left-hand side of inequality (9) approaches 1 as $L \to \infty$ (thus the inequality is satisfied) if the number of the solutions $M$ is $\mathcal{O}(1)$. Furthermore, it seems reasonable to assume that

$$\mathcal{L}_0(L) \geq L$$

(11)

because the index register requires $L$ qubits, and more qubits may be required for the oracle, the conditional phase shift, and so on. As we will show in this paper, macroscopically entangled states of size $\mathcal{O}(L)$ indeed appear during the computation if $M = \mathcal{O}(1)$.

Note that we are considering quantum computers which have almost the minimum number $\mathcal{L}(L)$ of qubits to perform $\mathcal{A}$. This is because it is generally possible to mask macroscopic entanglement if one can add arbitrarily many qubits to the computer. We exclude such uninteresting possibility by imposing Eq. (10). However, it is worth mentioning that one can easily generalize the above conjecture to the case where a quantum error correction [24] is used in the computer. That is, although the number of physical qubits does not satisfy Eq. (10) in such a case, one can identify each logical qubit with a large qubit. Then, Eq. (10) is satisfied for the number of the large qubits, and the conjecture can be applied if the macroscopic entanglement is defined in terms of the large qubits.

Since we only consider pure states in this paper, a macroscopically entangled state is a state with $p = 2$. Hence, the above conjecture may be stated roughly as follows: A quantum algorithm that is much faster than classical algorithms utilizes some state(s) with $p = 2$. Note that this does not claim that all states with $p = 2$ would be useful to fast quantum computation. In particular, the conjecture does not claim that all macroscopically entangled states appearing in the computation would be relevant to fast quantum computation. This point will be discussed in Secs. [VII] and [VIII] by showing examples.

Furthermore, the following fact is worth mentioning. For some macroscopically entangled states of size $L$, there are quantum circuits that convert a product state into such a state in $\mathcal{O}(L)$ steps if the target state with $p = 2$ is known when the circuits are designed. This fact has nothing to do with our conjecture. The point is that in quantum computation the states that appear at, e.g., the middle point of the computation are unknown when the circuits are designed, because the states depend on the solutions of the problems to be solved. The above conjecture claims the appearance of macroscopically entangled states in this case.

IV. ANALYTIC RESULTS FOR GROVER’S QUANTUM SEARCH ALGORITHM

Consider the problem of finding a solution to the equation $f(x) = 1$ among $N = 2^L$ possibilities, where $f(x)$ is a function, $f : \{0, 1\}^L \to \{0, 1\}$. If the number $M$ of solutions is $\mathcal{O}(1)$, this ‘search problem’ is hard in the sense that classical algorithms take $\mathcal{O}(N)$ steps. A quantum computer using Grover’s quantum search algorithm solves this problem much faster, with $\mathcal{O}(\sqrt{N})$ steps [18], and inequality (9) is satisfied. Hence, Grover’s algorithm is a representative quantum algorithm for unstructured problems [11]. We investigate the index $p$ of quantum states
appearing in a quantum computer that performs this algorithm. As a quantum computer, we consider the index register of $L$ qubits, and thus Eq. (10) is clearly satisfied. Suppose that the equation $f(x) = 1$ has $M$ solutions $x_1, \cdots, x_M$. If we put

$$|\alpha\rangle = \frac{1}{\sqrt{N-M}} \sum_{x \neq x_1, \cdots, x_M} |x\rangle,$$

$$|\beta\rangle = \frac{1}{\sqrt{M}} \sum_{x = x_1, \cdots, x_M} |x\rangle,$$

then the state $|\psi_0\rangle$ just after the first Hadamard transformation (see Eq. (30) below) is represented as

$$|\psi_0\rangle = \cos \frac{\theta}{2} |\alpha\rangle + \sin \frac{\theta}{2} |\beta\rangle.$$

Here, the angle $\theta$ is given by

$$\cos \frac{\theta}{2} = \sqrt{\frac{N-M}{N}}.$$

The Grover iteration $\hat{G} = (2|\psi_0\rangle\langle\psi_0| - I)\hat{O}$, where $\hat{O}$ denotes the oracle operator, performs the rotation by angle $\theta$ in the direction $|\alpha\rangle \rightarrow |\beta\rangle$ in the two-dimensional subspace spanned by $|\alpha\rangle$ and $|\beta\rangle$. The state $|\psi_k\rangle$ after $k$ ($= 0, 1, 2, \cdots$) iterations is therefore given by

$$|\psi_k\rangle = \hat{G}^k |\psi_0\rangle = \cos \left(\frac{2k+1}{2} \theta\right) |\alpha\rangle + \sin \left(\frac{2k+1}{2} \theta\right) |\beta\rangle.$$

Hence, by repeating the Grover iteration

$$R \equiv \left\lceil \frac{\arccos \sqrt{\frac{M}{N}}}{\theta} \right\rceil$$

times, one can find a solution to the search problem with probability $\geq 1/2$. Here, $[a]$ denotes the smallest integer among those larger than or equal to $a$. When $M \ll N$, in particular, we have $\theta \simeq 2\sqrt{M/N}$ and

$$R \simeq \left\lceil \frac{\pi}{4} \sqrt{\frac{N}{M}} \right\rceil.$$

A. When $M = 1$

When $M = 1$, Eqs. (12) and (13) reduce to $|\alpha\rangle = |\psi_0\rangle + O(1/\sqrt{N}) = |\psi_0\rangle + O(1/2L/2)$ and $|\beta\rangle = |x_1\rangle$, respectively. Since $|\psi_0\rangle$ and $|x_1\rangle$ are product states, we find that $p = 1$ for $|\psi_0\rangle$, $|\alpha\rangle$ and $|\beta\rangle$. For $|\psi_k\rangle$, on the other hand, Eq. (16) gives the expectation value of the ‘$x$ component of the magnetization’ $M_x = \sum_l \hat{\sigma}_x(l)$ as

$$\langle \psi_k | \hat{M}_x | \psi_k \rangle = \cos^2 \left(\frac{2k+1}{2} \theta\right) L + O(1).$$

On the other hand,

$$\langle \psi_k | \hat{M}_x^2 | \psi_k \rangle = \cos^2 \left(\frac{2k+1}{2} \theta\right) L^2 + O(L).$$

Equations (16) and (20) yield

$$\langle \psi_k | (\Delta \hat{M}_x)^2 | \psi_k \rangle = \frac{1}{4} \sin^2 (2k+1) \theta) L^2 + O(L).$$

We thus find that $\langle \psi_k | (\Delta \hat{M}_x)^2 | \psi_k \rangle = O(L^2)$, i.e., $p = 2$, if

$$\sin^2 ((2k+1) \theta) = O(1).$$
In a similar manner, we can also show that \( \langle \psi_k | (\Delta \hat{M}_z)^2 | \psi_k \rangle = \mathcal{O}(L^2) \), where \( \hat{M}_z = \sum_l \hat{\sigma}_z(l) \), for these states. \( \) In order to show that \( p = 2 \) for \( |\psi_k\rangle \), it is sufficient to find one additive observable which fluctuates macroscopically, as seen from the definition \( [2] \).

Since \( \theta \simeq 2/\sqrt{N} \), condition \( [22] \) is satisfied for all \( k \) such that

\[
\delta \leq \frac{4k + 2}{\sqrt{N}} \leq \pi - \delta, \tag{23}
\]

where \( \delta \) is an arbitrary small positive constant independent of \( N \). For example, all \( k \)'s such that \( 0.1R \leq k \leq 0.9R \) satisfy this condition, according to Eq. \( [15] \). We therefore conclude that most \( |\psi_k\rangle \)'s in the Grover iteration processes are entangled macroscopically (i.e., \( p = 2 \)) when \( M = 1 \), whereas \( p = 1 \) for the initial and final states.

Note that the above result explicitly shows that \( p \) is well defined for \( |\psi_k\rangle \)'s, although they are not strictly homogeneous in general. We say this fact as ‘\( |\psi_k\rangle \)'s are effectively homogeneous,’ as in Refs. [4, 11, 13].

### B. When \( M = \mathcal{O}(1) \)

When \( M = \mathcal{O}(1) \) and \( M \geq 2 \), we have \( |\alpha\rangle = |\psi_0\rangle + \mathcal{O}(1/\sqrt{N}) = |\psi_0\rangle + \mathcal{O}(1/2^{L/2}) \) and \( |\beta\rangle = (|x_1\rangle + \cdots + |x_M\rangle) / \sqrt{M} \). Since \( |\psi_0\rangle \) is a product state, \( p = 1 \) for \( |\psi_0\rangle \) and \( |\alpha\rangle \). However, unlike the case of \( M = 1 \), \( |\beta\rangle \) can have \( p = 2 \). For example, suppose that \( M = 2 \) and the two solutions are \( x_0 \equiv 1010 \cdots 10 \) and \( x_1 \equiv 0101 \cdots 01 \). Then, \( |\beta\rangle = (|x_0\rangle + |x_1\rangle) / \sqrt{2} \) is a state with \( p = 2 \) because \( \langle \beta | (\Delta \hat{M}_z)^2 | \beta \rangle = \mathcal{O}(L^2) \), where \( \hat{M}_z = \sum_l (1-l)^2 \hat{\sigma}_z(l) \).

For \( |\psi_k\rangle \) with \( k \geq 1 \), on the other hand, Eqs. \( [19] - [21] \) hold also in this case. Hence, the discussion including Eqs. \( [22] \) and \( [23] \) holds also. Therefore, we conclude that most \( |\psi_k\rangle \)'s in the Grover iteration processes are entangled macroscopically, i.e., \( p = 2 \), when \( M = \mathcal{O}(1) \), whereas \( p = 1 \) for the initial state. For the final state, \( p \) depends on the nature of the solutions.

### C. When \( M = \mathcal{O}(N) \)

The case of \( M = \mathcal{O}(1) \) is most important and interesting because condition \( [4] \) is clearly satisfied. In contrast, the cases of large \( M \) such as \( M = \mathcal{O}(\sqrt{N}) \) and \( M = \mathcal{O}(N) \) are uninteresting because condition \( [4] \) is not satisfied. For completeness, however, we briefly discuss the case of \( M = \mathcal{O}(N) \) as an example of such uninteresting cases.

When \( M = \mathcal{O}(N) \), Grover’s algorithm does not necessarily use macroscopically entangled states. For example, suppose that \( N \) is a multiple of 8 and all multiples of 8 less than \( N \) are solutions. Then,

\[
|\alpha\rangle = \sqrt{\frac{8}{7N}} \sum_{y=0}^{N/8-1} \sum_{z=1}^7 |yz\rangle = \sqrt{\frac{1}{7}} \sum_{z=1}^7 | \rightarrow \cdots \rightarrow z \rangle, \tag{24}
\]

\[
|\beta\rangle = \frac{\sqrt{8}}{N} \sum_{y=0}^{N/8-1} |y000\rangle = | \rightarrow \cdots \rightarrow 000 \rangle, \tag{25}
\]

where \( | \rightarrow \rangle = (|0\rangle + |1\rangle) / \sqrt{2} \). Hence, all \( |\psi_k\rangle \)'s are product states except for the last three qubits. Since entanglement of \( \mathcal{O}(1) \) qubits cannot be the macroscopic entanglement, we find that \( p = 1 \) for all \( |\psi_k\rangle \)'s. This does not contradict with the conjecture of Sec. IIII because condition \( [4] \) is not satisfied when \( M = \mathcal{O}(N) \).

### D. Relevance of macroscopic entanglement to faster computation by Grover’s algorithm

From the results of Secs. IV A and IV B we confirm the conjecture of Sec. IIII for Grover’s quantum search algorithm, at least for the most important case of \( M = \mathcal{O}(1) \). On the other hand, as mentioned in Sec. IIII the conjecture does not claim that all macroscopically entangled states appearing in the computation would be essential to fast quantum computation. We now study this point.

When \( M = \mathcal{O}(1) \), we have seen that most \( |\psi_k\rangle \)'s such that inequality \( [23] \) is satisfied are entangled macroscopically (i.e., \( p = 2 \)), whereas the final state \( |\psi_R\rangle \) may or may not be so depending on the number and natures of the solutions. This fact suggests the following: The macroscopic entanglement of most \( |\psi_k\rangle \)'s should be relevant to the speedup by Grover’s algorithm, whereas the macroscopic entanglement of the final state (and states close to the final state) should be irrelevant. We argue that this is indeed the case.
In a similar manner, we can show that the macroscopic entanglement of most \( |\psi_k\rangle \)'s is crucial to faster computation. Therefore, the macroscopic entanglement of \( |\psi_k\rangle \)'s is sufficient for confirming our conjecture, we now study entanglement not only of \( |\psi_k\rangle \)'s but also of such \( |\psi_k\rangle \)'s but also of such intermediate states in order to see details of evolution of entanglement. For this purpose, we numerically simulate a quantum computer that performs Grover’s quantum search algorithm. As in the previous section, we consider the index register of \( L \) qubits as a quantum computer, and thus Eq. \( (10) \) is clearly satisfied.

### V. NUMERICAL RESULTS FOR GROVER’S QUANTUM SEARCH ALGORITHM

In the analysis of Sec. IV, we have considered entanglement of \( |\psi_k\rangle = \hat{G}^k |\psi_0\rangle \ (k = 0, 1, 2, \ldots, R) \). In actual quantum computations, the Grover iteration \( \hat{G} \) is realized as a series of local and pair-wise operations. Hence, many intermediate states appear during the steps between \( |\psi_k\rangle \) and \( |\psi_{k+1}\rangle \). Although the macroscopic entanglement of \( |\psi_k\rangle \)'s is sufficient for confirming our conjecture, we now study entanglement not only of \( |\psi_k\rangle \)'s but also of such intermediate states in order to see details of evolution of entanglement. For this purpose, we numerically simulate a quantum computer that performs Grover’s quantum search algorithm. As in the previous section, we consider the index register of \( L \) qubits as a quantum computer, and thus Eq. \( (10) \) is clearly satisfied.

#### A. Formulation of simulation

We simulate the case of \( M = 1 \) because this case is most fundamental in the search problem. The solution \( x_1 \) is chosen randomly. We have confirmed that this random choice of a solution makes no significant differences on the results of the numerical simulations presented below.

As the initial state, a register \( \mathcal{R} \) composed of \( L \) qubits is set to be the following product state;

\[
|\psi_{\text{init}}\rangle = |0\rangle.
\]

(29)

Firstly, the Hadamard transformation is performed by successive applications of the Hadamard gate on individual qubits in \( \mathcal{R} \), and the quantum state evolves into

\[
|\psi_0\rangle = \frac{1}{\sqrt{2^L}} \sum_{x=0}^{2^L-1} |x\rangle.
\]

(30)

Then we apply the Grover iteration \( \hat{G} = (2|\psi_0\rangle\langle\psi_0| - |\rangle\langle\rangle) \hat{O} \), which consists of two Hadamard transformations, an oracle operation \( \hat{O} \), and a conditional phase shift \( \hat{P} \), which works as

\[
\hat{P}|0\rangle = |0\rangle,
\]

\[
\hat{P}|x\rangle = -|x\rangle \quad (x > 0).
\]

(31)

(32)
Each Hadamard transformation requires $L$ operations of the Hadamard gate. The oracle $\hat{O}$ is constructed depending on the function $f(\cdot)$, and requires its own workspace qubits and computational steps. However, since the oracle is not a proper part of the Grover’s algorithm, we simulate the operation of $\hat{O}$ as a one-step operation, and its workspace is not included in the simulation. The execution of the conditional phase shift $\hat{P}$ requires $O(L)$ pairwise unitary operations. For simplicity, we simulate $\hat{P}$ as a one-step operation. As a result, each Grover iteration is simulated by $2L + 2$ steps of operations. After the applications of the Grover iterations $R$ times, the state $|\psi_0\rangle$ evolves to

$$\hat{G}^R|\psi_0\rangle = |\psi_R\rangle \simeq |x_1\rangle.$$  

(33)

Finally, by performing a measurement on $R$, one can obtain the solution $x_1$ with a sufficiently high probability. We do not simulate this measurement process. The total computational steps $Q(L)$ in our simulation is thus

$$Q(L) = L + (2L + 2)R = O(\sqrt{2L}).$$  

(34)

B. Results of simulation

Figure 1 plots $e_{\text{max}}$ along the steps of Grover’s algorithm, for $L = 8, 9, 10, 12, 14$ when $x_1 = 19, 388, 799, 1332, 9875$, respectively. Figure 2 is a magnification from the 1st to 40th steps for $L = 8$, whereas a magnification from the 1005th to 1155th steps for $L = 14$ is shown in Fig. 3.

FIG. 1: The maximum eigenvalue $e_{\text{max}}$ of the VCM of quantum states appearing in Grover’s quantum search algorithm for $L = 8, 9, 10, 12, 14$ when $x_1 = 19, 388, 799, 1332, 9875$, respectively, as functions of the step of the algorithm. The horizontal line represents the value of $e_{\text{max}}$ for product states, $e_{\text{max}} = 2.00$.

It is seen that $e_{\text{max}} = 2.00$ for all states from $|\psi_{\text{init}}\rangle$ to $|\psi_0\rangle$, i.e., during the initial Hadamard transformation, which is denoted as ‘HT’ from the 1st to 8th steps in Fig. 2. This is because all these states are product states, for which we can easily show that $e_{\text{max}} = 2$ (Appendix B). When the stage of Grover iterations begins, $e_{\text{max}}$ grows gradually, as seen from Figs. 1 and 2. In each Grover iteration, Figs. 2 and 3 show that $e_{\text{max}}$ changes when $\hat{O}$ is operated, whereas it is kept constant during the subsequent Hadamard transformation. Then, it changes again when $\hat{P}$ is operated, whereas it is kept constant again during the subsequent Hadamard transformation. As the Grover iterations are repeated, $e_{\text{max}}$ continues to increase as a whole, until it takes the maximum value after about $R/2$ times applications of $\hat{G}$. Further applications of $\hat{G}$ reduce $e_{\text{max}}$, as seen from Fig. 1, toward $e_{\text{max}} \simeq 2.00$ for $|\psi_R\rangle$, which is approximately a product state as seen from Eq. (33).

To determine $p$, we note that $e_{\text{max}}$’s are of the same order of magnitude for all states from $|\psi_k\rangle$ to $|\psi_{k+1}\rangle$ for each $L$, as seen from Figs. 2 and 3. Hence, they have the same value of $p$ as $|\psi_k\rangle$. Therefore, from the result of the
previous section, we conclude that all states from $|\psi_k\rangle$ to $|\psi_{k+1}\rangle$ have $p = 2$ for all $k$ which satisfies inequality (23). As a demonstration, we plot $e_{\text{max}}$’s of $|\psi_{\lfloor R/2 \rfloor}\rangle$, $|\psi_{\lfloor R/3 \rfloor}\rangle$ and $|\psi_{\lfloor R/4 \rfloor}\rangle$ in Fig. 4 as functions of $L$. Since $e_{\text{max}}$’s are all proportional to $L$, we can confirm that $p = 2$, i.e., these states are entangled macroscopically. Note that Fig. 4 also demonstrates again that $p$ is well defined, although the states are not strictly homogeneous.
FIG. 4: $e_{\text{max}}$'s of $|\psi_{R/2}\rangle$ (diamonds), $|\psi_{R/3}\rangle$ (crosses) and $|\psi_{R/4}\rangle$ (squares), as functions of $L$. The dotted lines are the guides to the eyes, whereas the horizontal line represents the value of $e_{\text{max}}$ for product states, $e_{\text{max}} = 2.00$.

C. Summary of analyses of Grover’s quantum search algorithm

The results of Secs. IV and V for Grover’s quantum search algorithm, which is a representative algorithm for unstructured problems, are summarized as follows.

When the number of solutions $M = \mathcal{O}(1)$, the search problem is hard in the sense that classical algorithms take $\mathcal{O}(N)$ steps. This case is most important and interesting because condition (9) is clearly satisfied. In this case, we have shown that most $|\psi_k\rangle$’s in Grover’s algorithm are entangled macroscopically ($p = 2$), and thus the conjecture of Sec. III is confirmed.

We have also found that the final state $|\psi_R\rangle$ may or may not be so depending on the number and natures of the solutions. The conjecture does not claim that all macroscopically entangled states appearing the computation would be relevant to fast quantum computation. We have shown that the macroscopic entanglement of most $|\psi_k\rangle$’s is crucial to faster computation, whereas that of the final state is irrelevant.

The cases of large $M$ such as $M = \mathcal{O}(\sqrt{N})$ and $M = \mathcal{O}(N)$ are uninteresting in view of quantum computation because condition (10) is not satisfied. For completeness, we briefly discuss the case of $M = \mathcal{O}(N)$ as an example of such uninteresting cases, and have shown that Grover’s algorithm does not necessarily use macroscopically entangled states.

VI. ANALYSIS OF SHOR’S FACTORING ALGORITHM

In this section, we study Shor’s factoring algorithm [16, 17], as a representative algorithm for structured problems [1].

A. Formulation of simulation

Let $N$ be a positive integer to be factored, $x$ a random number co-prime to $N$ which satisfies $0 < x < N$, and $r$ the ‘order,’ i.e., the least positive integer which satisfies $x^r \equiv 1 \pmod{N}$. For a given pair of $N$ and $x$, one can find the value of $r$ efficiently using Shor’s algorithm. The first and second registers are denoted by $\mathcal{R}_1$ and $\mathcal{R}_2$, respectively, which have $L$ and $L'$ qubits. We take [23]

$$\log_2 N \leq L' \leq \log_2 N + 1, \quad L = 2L'.$$  (35)
We assume that this model satisfies Eq. (10). Note, however, that even if \( R_2 \) could be replaced with a shorter register, the main result of this section would not change because, as shown below, only the qubits of \( R_1 \) are entangled macroscopically.

The initial state \( |\psi_{\text{init}}\rangle \) is the product of two product states \( |0\rangle^{(1)} \) and \( |1\rangle^{(2)} \) of \( R_1 \) and \( R_2 \), respectively. We denote by \( |\psi_{\text{HT}}\rangle \), \( |\psi_{\text{ME}}\rangle \), and \( |\psi_{\text{DFT}}\rangle \) the states just after the Hadamard transformation, modular exponentiation (ME), and discrete Fourier transformation (DFT), respectively. For the DFT, we employ the quantum circuit of Sec. V of Ref. [17], which costs \( L(L + 1)/2 \) steps. The final states is \( |\psi_{\text{DFT}}\rangle \).

As in Ref. [4], we represent the process \( |\psi_{\text{HT}}\rangle \rightarrow |\psi_{\text{ME}}\rangle \) simply as the product of \( L \) controlled unitary transformations, because \( R_1 \) takes a major role [4]. As a result, the states appearing during the modular exponentiation in our simulations correspond to \( L \) representative states out of \( \mathcal{O}(L^3) \) states. As a result of this simplification, the total number \( Q(L) \) of computational steps in our simulation becomes

\[
Q(L) = 2L + \frac{L(L + 1)}{2},
\]

which is smaller than \( \mathcal{O}(L^3) \) steps of a real computation. To find the macroscopic entanglement, we shall evaluate \( e_{\max} \) of the states that appear during the computation, as a function of \( L_{\text{tot}} = L + L' = 3L/2 \). [Since \( L_{\text{tot}} = \mathcal{O}(L) \), we will obtain the same results for \( p \) if we evaluate \( e_{\max} \) as a function of \( L \).]

### B. Results of the simulation

Figure 5 plots the maximum eigenvalue \( e_{\max} \) of the VCM along the steps of the algorithm, when \( N = 21, L_{\text{tot}} = 15, x = 2 \), for which \( r = 6 \). It is seen that \( e_{\max} = 2.00 \) for all states from \( |\psi_{\text{init}}\rangle \) to the end of the Hadamard transformation. This is because all these states are product states, for which \( e_{\max} = 2 \) (Appendix B). When the stage of the modular exponentiation begins, \( e_{\max} \) grows, until it becomes 5.00 for \( |\psi_{\text{ME}}\rangle \). Then, throughout the stage of the discrete Fourier transformation, \( e_{\max} \) keeps large values, slightly changing step by step.

![FIG. 5: \( e_{\max} \) of quantum states appearing in Shor’s factoring algorithm when \( N = 21, L_{\text{tot}} = 15, x = 2 \), for which \( r = 6 \), as a function of the step of the algorithm.](image)

For other values of \((N, x)\), and thus for other values of \( L_{\text{tot}} \) according to Eq. (35), we find that \( e_{\max} \) behaves similarly if \((N, x)\) gives \( r = 6 \). For example, Fig. 6 plots \( e_{\max} \) when \( N = 104, x = 55 \), for which \( r = 6 \) again, and \( L_{\text{tot}} = 21 \). It is seen that \( e_{\max} \) behaves similarly to the case of Fig. 5. Therefore, as in Ref. [4], we study the dependence of \( e_{\max} \) on \( L_{\text{tot}} \) by varying \((N, x)\) under the condition that it gives the same value of the order \( r, r = 6 \). In this case, the states in Shor’s algorithm become effectively homogeneous for which \( p \) is well defined, as shown in Ref. [4] and in the following.
FIG. 6: $\epsilon_{\text{max}}$ of quantum states appearing in Shor’s factoring algorithm when $N = 104$, $L_{\text{tot}} = 21$, $x = 55$, for which $r = 6$, as a function of the step of the algorithm.

Figure 7 plots the $L_{\text{tot}}$ dependence of $\epsilon_{\text{max}}$ that is calculated in this way for three representative states including $|\psi_{\text{ME}}\rangle$, the state at the $\frac{L}{2} (\frac{L}{2} + 1)$-th step of the DFT stage (i.e., just after the pair-wise unitary transformations targeting $L/2$ qubits of $R_1$ are finished), and the final state $|\psi_{\text{DFT}}\rangle$. For each state, $\epsilon_{\text{max}}$ increases linearly with increasing $L_{\text{tot}}$. Therefore, $p = 2$ for these states. In a similar manner, we find that all states after the modular exponentiation have $p = 2$ for $r = 6$, i.e., they are macroscopically entangled. We have also obtained the same conclusion for other values of $r$ ranging from 2 to 20, except when $r$ becomes an integral power of 2 (i.e., $r = 2, 4, 8, 16$), for which we find that states with $p = 2$ are not necessarily used.

Note that we already found in the previous work [4] that the two states, $|\psi_{\text{ME}}\rangle$ and $|\psi_{\text{DFT}}\rangle$, are macroscopically entangled by studying specific additive operators. In the present work, in contrast, we have proved the macroscopic entanglement of all states after the modular exponentiation, by surveying all possible additive operators by the VCM method. This demonstrates the power of the VCM method.

Another advantage of the VCM method is that one can identify the maximally-fluctuating additive operator(s) from the eigenvector(s) corresponding to $\epsilon_{\text{max}}$. For example, $|\psi_{\text{ME}}\rangle$ for $r = 6$ have two degenerate eigenvectors corresponding to $\epsilon_{\text{max}}$, from which we find that the following two operators are the maximally-fluctuating additive operators:

$$\hat{A}_{\text{max}} = \sqrt{\frac{3}{2}} \sum_{l=2}^{L} (-1)^{l} \hat{\sigma}_{y}(l),$$  \hspace{1cm} (37)$$

$$\hat{A}'_{\text{max}} = \sqrt{\frac{3}{2}} \sum_{l=2}^{L} \hat{\sigma}_{x}(l).$$  \hspace{1cm} (38)$$

For other values of $r$, other operators become the maximally-fluctuating additive operators. In particular, the absence of operators of $l = 1$ in Eqs. (37) and (38) are accidental, i.e., such operators are included in the sums of the maximally-fluctuating additive operators for other values of $r$. Note that $A_{\text{max}}$ and $A'_{\text{max}}$ do not contain operators of the second register $R_2$. This fact shows that the first register $R_1$ are entangled macroscopically, whereas $R_2$ is not, in consistency with the result of Ref. [4].
FIG. 7: $e_{\text{max}}$ of $|\psi_{\text{ME}}\rangle$ (diamonds), the state at the $L/4 (L/2 + 1)$-th step of the DFT stage (squares), and the final state $|\psi_{\text{DFT}}\rangle$ (crosses), for $r = 6$, as functions of $L_{\text{tot}} = L + L' = 3L/2$. The horizontal line represents the value of $e_{\text{max}}$ for product states, $e_{\text{max}} = 2.00$.

C. Simulation with measurement after the modular exponentiation

In the above simulations of Shor’s algorithm, measurement is not performed during the quantum computation. In the original paper by Shor [16], on the other hand, measurement diagonalizing the computational basis is performed on $\mathcal{R}_2$ when the stage of the modular exponentiation is finished [17]. We also simulate this case.

Figure 8 plots $e_{\text{max}}$ under the same condition as Fig. 5 except that the measurement is performed at the end of the modular exponentiation. By the measurement, the state of $\mathcal{R}_2$ is determined to be one of the states $|x \mod N \rangle^{(2)}$ where $a = 1, 2, \cdots, r$. Therefore, $e_{\text{max}}$ can take $r$ different profiles after the measurement. Only two different profiles of $e_{\text{max}}$ appear in Fig. 8 because those for $a = 1, 2, 3, 4$ happen to be identical and those for $a = 5, 6$ happen to be identical. Both profiles of $e_{\text{max}}$ are quite similar to the profile of Fig. 5. Therefore, the measurement on $\mathcal{R}_2$ at the end of the modular exponentiation does not suppress the macroscopic entanglement.

D. Relevance of macroscopic entanglement to faster computation by Shor’s algorithm

We have found that in Shor’s factoring algorithm all states after the modular exponentiation are macroscopically entangled for almost all nontrivial values of $(N, x)$, i.e., except for the special case where their values are such that the order $r$ becomes an integral power of 2. [This exceptional case will be discussed again in Sec. VII] This again supports the conjecture of Sec. III.

However, as in the Grover’s algorithm, this does not mean that all of such states could be relevant to the faster computation. In fact, we already showed in Ref. [4] that the macroscopic entanglement of the final state $|\psi_{\text{DFT}}\rangle$ is irrelevant to the faster computation, whereas that of $|\psi_{\text{ME}}\rangle$ is crucial. This crucial macroscopic entanglement of $|\psi_{\text{ME}}\rangle$ does not disappear even if measurement is performed on the second register just after the modular exponentiation is finished. Therefore, as in the Grover’s algorithm, macroscopic entanglement plays an essential role in Shor’s factoring algorithm.

VII. DISCUSSIONS AND CONCLUSIONS

We have investigated macroscopic entanglement of quantum states in quantum computers that perform Grover’s quantum search algorithm and Shor’s factoring algorithm. Here, we say a state is entangled macroscopically iff it has
FIG. 8: $\epsilon_{\text{max}}$ of quantum states appearing in Shor’s factoring algorithm with measurement of the second register at the end of the modular exponentiation, when $N = 21$, $L_{\text{tot}} = 15$, $x = 2$, for which $r = 6$, as a function of the step of the algorithm. After the measurement, denoted by the asterisk, two different profiles of $\epsilon_{\text{max}}$ appear depending on the outcome of the measurement.

superposition of macroscopically states. As a well-defined index of macroscopic entanglement, we have employed the index $p$ that was proposed and studied in Refs. [12]. Using the method developed in Ref. [12], we have calculated this index as a function of the step of each algorithm.

For both algorithms, we have found that whether macroscopically entangled states are used or not depends on the numbers and properties of the solutions to the problem to be solved. When the solutions are such that the problem becomes hard in the sense that classical algorithms take more than polynomial steps to find a solution, macroscopically entangled states are always used in Grover’s algorithm and used almost always (i.e., except when the order $r$ is an integral power of 2) in Shor’s algorithm.

Since Grover’s and Shor’s algorithms are representative ones for unstructured and structured problems, respectively, our results support strongly the conjecture (see Sec. III) that quantum computers should utilize macroscopically entangled states that is defined by $p$ in some stages of the computation when they solve hard problems much faster than any classical algorithms.

Note that there are many different states with $p = 2$ in many-qubit systems. Which ones are used depends on the quantum algorithms and the inputs. Note in particular that this conjecture does not claim that all states with $p = 2$ would be useful in quantum computation. Furthermore, among states with $p = 2$ that do appear during quantum computation, some can be irrelevant to efficient computation, as discussed in Secs. IV D and V D and in Ref. [4].

It is interesting to take the contraposition of the conjecture, i.e., if macroscopically entangled states are not used throughout a quantum algorithm which satisfies Eq. (17), then there must exist a classical algorithm that can solve the problem as efficiently as the quantum algorithm, i.e., inequality (8) is not satisfied. This may be used to explore classical algorithms with the help of knowledge about quantum algorithms. For example, we have found that Shor’s factoring algorithm does not necessarily use macroscopically entangled states in the exceptional case where the order $r$ is an integral power of 2. According to the above contraposition, this suggests that there would exist a classical algorithm that efficiently solve the problem in this special case.

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APPENDIX A: RANGE OF $p$

The range of $p$ is $1 \leq p \leq 2$. For a system composed of $L$ qubits, this can easily be shown as follows [23]. Let $e_1, e_2, \cdots$ be the eigenvalues of the variance-covariance matrix $V$, Eq. (B3), which is a $3L \times 3L$ non-negative hermitian matrix. Since $\sum_{\alpha} \langle \psi(L) | (\Delta \hat{\sigma}_\alpha(l))^2 | \psi(L) \rangle = O(1)$ for every $|\psi(L)\rangle$ and $l$, we find

$$3L e_{\text{max}}(L) \geq \sum_i e_i = \text{Tr} V = \sum_l \sum_{\alpha} \langle \psi(L) | (\Delta \hat{\sigma}_\alpha(l))^2 | \psi(L) \rangle = O(L). \quad (A1)$$

Therefore, according to Eq. (7), $p \geq 1$. On the other hand, $p \leq 2$ because

$$\left| \langle \psi(L) | \Delta \hat{A}^\dagger \Delta \hat{A} | \psi(L) \rangle \right| \leq \sum_l \sum_{\alpha, \alpha'} \left| \langle \psi(L) | \hat{c}_{\alpha l} \Delta \hat{\sigma}_\alpha(l) \hat{c}_{\alpha' l'} \Delta \hat{\sigma}_{\alpha'}(l') | \psi(L) \rangle \right| \leq O(L^2). \quad (A2)$$

These arguments can be easily generalized to more general systems.

APPENDIX B: MAXIMUM EIGENVALUE OF THE VCM FOR PRODUCT STATES

In this appendix, we show that $e_{\text{max}} = 2$ for a pure state $|\psi\rangle$ if it is a product state,

$$|\psi\rangle = \bigotimes_{l=1}^{L} |\phi_l\rangle_l, \quad (B1)$$

where $|\phi_l\rangle_l$ denotes a state of the qubit at site $l$ ($= 1, 2, \cdots, L$). The VCM of such a state becomes a block-diagonal matrix

$$
\begin{pmatrix}
V_1 & 0 & \cdots & 0 \\
0 & V_2 & \cdots & 0 \\
\vdots & 0 & V_3 & \cdots \\
0 & \cdots & \cdots & 0 \\
\end{pmatrix}, \quad (B2)
$$

where $V_l$ is a $3 \times 3$ matrix whose $\alpha\beta$ element ($\alpha, \beta = x, y, z$) is given by

$$
(V_l)_{\alpha\beta} = \langle \psi | \hat{\sigma}_\alpha(l) \hat{\sigma}_\beta(l) | \psi \rangle - \langle \psi | \hat{\sigma}_\alpha(l) \rangle \langle \psi | \hat{\sigma}_\beta(l) \rangle. \quad (B3)
$$

Therefore, $e_{\text{max}}$ is given by the maximum one among the maximum eigenvalues of $V_l$'s. By a unitary transformation of this $3 \times 3$ matrix such that $|\phi_l\rangle$ becomes an eigenstate of the transformed $\hat{\sigma}_z(l)$, we can transform $V_l$ into

$$
V_l = \begin{pmatrix}
1 & i & 0 \\
-i & 1 & 0 \\
0 & 0 & 0 \\
\end{pmatrix}. \quad (B5)
$$

Since the maximum eigenvalue of this matrix is 2, we find that $e_{\text{max}} = 2$.

[1] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, 2000).
[2] G. Vidal, Phys. Rev. Lett. 91, 147902 (2003)
[3] R. Jozsa and N. Linden, Proc. R. Soc. London, Ser. A 459, 2011 (2003)
[4] A. Ukena and A. Shimizu, Phys. Rev. A 69, 022301 (2004).
[5] C. H. Bennett, S. Popescu, D. Rohrlich, J. A. Smolin, and A. V. Thapliyal, Phys. Rev. A 63, 012307 (2000).
[6] A. Miyake and M. Wadati, Phys. Rev. A 64, 042317 (2001).
[7] D. A. Meyer and N. R. Wallach J. Math. Phys. 43(9), 4273 (2002).
Although this might sound strange to the reader who is not familiar with quantum theory of infinite systems, its physics may be understood as follows. Consider a cat state $|\psi(L)\rangle \equiv (|00\cdots0\rangle + |11\cdots1\rangle)/\sqrt{2}$ of size $L$ as the simplest example. If $L$ is finite, there exist observables that have non-vanishing matrix elements between $|00\cdots0\rangle$ and $|11\cdots1\rangle$. The expectation values of such observables discriminate between the pure state $|\psi(L)\rangle$ and the mixed state $ho(L) \equiv (|00\cdots0\rangle\langle00\cdots0| + |11\cdots1\rangle\langle11\cdots1|)/2$. If we take the $L \to \infty$ limit, on the other hand, quantum theory of infinite systems require that every observables should be a function of field operators within a finite region in an infinite space. As a result, there are no observables that have non-vanishing matrix elements between the $L \to \infty$ limits of $|00\cdots0\rangle$ and $|11\cdots1\rangle$. This implies that $\lim_{L \to \infty} |\psi(L)\rangle$ is not a pure state. More mathematically speaking, $\lim_{L \to \infty} |\psi(L)\rangle$ is not a vector state of an irreducible representation. For details, see Ref. [11] and references cited therein.