

Thesis

Theory of quantum measurement of
energy

Quantum algorithm and its evaluation—
(エネルギーの量子測定理論-量子ア
ルゴリズムとその性能評価-)

by

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December 2013

Abstract

According to the axioms of quantum mechanics, there exists a quantum measurement corresponding to each observable. Energy is one of such observables, and the operator of the energy is called Hamiltonian. The Hamiltonian specifies the dynamics of closed quantum systems and it also characterizes the property of the equilibrium state in contact with a heat bath. Therefore the energy is an essential quantity in quantum mechanics, which characterizes behavior of a quantum system. On the other hand, since the Hamiltonian is not a local observable in general, a concrete construction of how to apply the quantum measurement of energy is not trivial. Thus various measurement models of energies have been proposed, and also discussions have been made on whether the time is a resource to be consumed to increase the precision of energy measurement in connection with the time-energy uncertainty relationship.

Constructing a way to implement the energy measurement on an unknown Hamiltonian system is important, since it avoids constructing a new measurement scheme for each new quantum system. On the other hand, among measurements of energy, the projective measurement of energy has useful properties for applications. The projective measurement is a measurement which satisfies the condition so-called *repeatable hypothesis* that when we measure the state immediately after obtaining an outcome from the same measurement, we obtain the same outcome again.

In this thesis, we consider two schemes to implement the projective measurement of energy for an unknown Hamiltonian system. One is a tomography based method, which is a construction suggested in the paper of Aharonov et. al. (2002). The other is the phase estimation based method, which utilizes the Hamiltonian dynamics of the system as a resource for the quantum algorithm, and realizes the projective measurement of energy on the system without identifying all parameters of the Hamiltonian. In this thesis, we assume there is a finite dimensional quantum system (quantum computer) which is able to apply any interaction between the target system and the finite dimensional system although the interaction should not depend on the target system Hamiltonian.

To evaluate the performance of the measurements implemented by the two schemes, we formulate two evaluation functions called *fluctuation of measurement value* and *non-repeatability*, which can evaluate how much a measurement is different from the ideal projective measurement of an observable. We calculate a sufficient time to guarantee the fluctuation of measurement value below some

small value ε , for each of the two measurement schemes. We find that the tomography based method takes the time proportional to $O(d^4 \Delta_{\max}/\varepsilon)$, while the phase estimation based method takes $O(\Delta_{\max}^3/\varepsilon^2)$, where d is the dimension of the target system and Δ_{\max} is the difference between the largest energy eigenvalue and the smallest energy eigenvalue. We show that the phase estimation based method performs better for large particle systems.

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Chapter 1

Introduction

According to the axioms of quantum mechanics, there exists a quantum measurement corresponding to each observable. Energy is one of such observables, and the operator of the energy is called Hamiltonian. The Hamiltonian specifies the dynamics of closed quantum systems and it also characterizes the property of the equilibrium state in contact with a heat bath. Therefore the energy is an essential quantity in quantum mechanics, which characterizes behavior of a quantum system. On the other hand, since the Hamiltonian is not a local observable in general, a concrete construction of how to apply the quantum measurement of energy is not trivial. Thus various measurement models of energies have been proposed [1, 2, 3, 4, 5], and also discussions have been made on whether the time is a resource to be consumed to increase the precision of energy measurement.

Among measurements of energy, the projective measurement of energy has useful properties for applications. The projective measurement is a measurement which satisfies the condition so-called *repeatable hypothesis* [6, 7] that when we measure the state immediately after obtaining an outcome from the same measurement, we obtain the same outcome again. Quantum non-demolition measurement (QND) is an example of the application of the projective measurement [8]. One type of QND is a sequence of projective measurement of energy on the same system, which is considered to be beyond the standard quantum limit that experimental confirmation of the gravity-wave detection faces. It will return the same outcome even when the measurements are separated by arbitrarily long intervals, as long as no external factor disturbs the system throughout the sequence. It makes the projective measurement of energy ideal for high-precision quantum metrology. Another application of the projective measurement of energy is for the experimental confirmation of the fluctuation theorem [9, 10, 11], which relates the probability of microscopic energy transition to macroscopic properties of energy, heat work in of the thermodynamics.

Most of the previous proposals for implementing the energy measurement on quantum systems work only when the Hamiltonians of quantum systems are known. Constructing a method to implement the energy measurement on unknown Hamiltonian systems is useful, since it can be performed on quantum systems by a fixed procedure which is independent from the Hamiltonian. The energy measurement on an unknown Hamiltonian system was once considered in [12], but still substantial progress is required for efficient implementation. In this thesis, we construct schemes to implement the projective measurement of energy on finite dimensional quantum systems with unknown Hamiltonians and analyze their running time required to guarantee a certain level of performance of energy measurement. We investigate how the running time depends on the dimension of the system. The Hamiltonian of the system is unknown but we only

require the difference between the minimum and the maximum eigenvalues of the system Hamiltonian is to be bounded and given by a known constant. Even if we consider the case that the bound is known, the number of parameters for identifying Hamiltonian is not reduced and implement the energy measurement is still non-trivial.

In this thesis, we consider two schemes to implement the projective measurement of energy for an unknown Hamiltonian system. One is a tomography-based method, which is a construction suggested in the paper of Aharonov et. al. (2002) [12, 13]. The other is the phase estimation based method, which utilizes the Hamiltonian dynamics of the system as a resource for the quantum algorithm, and realizes the projective measurement of energy on the system without identifying all parameters of the Hamiltonian. In this thesis, we assume there is a finite dimensional quantum system (quantum computer) which is able to apply any interaction between the target system and the finite dimensional system although the interaction should not depend on the target system Hamiltonian. The quantum computer works in enough short duration to ignore the dynamics caused by the self-Hamiltonian of the target system. Thus the total time of the measurement is evaluated by the sum of the idle times of the quantum computer, which causes a required time evolution on the target system before the next operation. In quantum information, *query complexity* [14] is the time cost determined by the number of use of an unknown unitary gate. For example, the cost of Grover's database search algorithm [15] is analyzed in terms of query complexity. Especially when the gate is given by the Hamiltonian dynamics, the time cost is called *Hamiltonian query* [16].

In the tomography-based method, we construct a linear estimation scheme of the unitary operation, and we takes the logarithm for the estimated operation to identify the Hamiltonian. However, the probability to return the result which has no physical counterpart is known to be a disadvantage of the linear estimation [17]. It is also the case with our estimator. The estimated operator can be a general complex matrix, on which the logarithm operation is not well-defined. We analyze this method on the assumption that there is an appropriate converter which deforms a given operator into a regular, normal matrix while leaving the statistical property of each element the same as the original operator.

In the phase estimation based method, our key contribution is to make Kitaev's phase estimation algorithm [18], which is used in Shor's factorization algorithm [19], applicable for our situation by presenting a new quantum algorithm called universal controllization. Kitaev's phase estimation algorithm had been shown to implement the projective measurement of energy in the asymptotic limit [20, 21]. To perform this algorithm, the Hamiltonian dynamics of the

target system has to be coherently controlled by the state of a memory qubit (control qubit). This means that if the state of a memory qubit is $|0\rangle$, the dynamics of the system is static, and if the state of the memory is $|1\rangle$, the dynamics of the system is applied as usual, and if the state is in the superposition of $|0\rangle$ and $|1\rangle$, the superposition of the two is realized. There were attempts [22, 23] to obtain the controlled dynamics for an unknown Hamiltonian dynamics; however there is a proof that the exact controllization is impossible in general [24]. (The methods of controllization presented by [22, 23] has turned out to be not applicable to completely unknown Hamiltonian dynamics). In this thesis, we construct a scheme of universal controllization which approximately realizes the controlled Hamiltonian dynamics, thereby avoiding the impossibility of exact implementation. In our new algorithm, the Hamiltonian dynamics is divided into a short time sequence and randomization processes are inserted between sequences. The resulting dynamics cancels emerging entanglement between the target system and the quantum computer which has the main obstacle for controllization of the unknown Hamiltonian.

To evaluate the performance of the measurements implemented by the two schemes, we formulate two evaluation functions called *fluctuation of measurement value* and *non-repeatability*, which can evaluate how much a measurement is different from the ideal projective measurement of an observable. Fluctuation of measurement value is defined as the mean squared error of the measurement outcome. non-repeatability evaluates how a measurement behaves differently from the repeatable hypothesis. These two are defined in a similar spirit as the error and the disturbance defined by Ozawa [26]. There are also two known evaluation methods of the distance between measurements, namely *Monge distance* [27, 30] for two probability distributions and *diamond norm* [33, 34] for two instruments (probabilistic maps) associated with the state changes for each outcome. In these two evaluation methods, measurement on not only eigenstates but also all possible states should be taken into account to evaluate the performance of the measurement. This arbitrariness of the states makes these methods very hard to calculate. The Monge distance includes the maximization over Lipschitz functions which is hard to calculate, and the diamond norm can not be well-defined in our situation. In this thesis, we formulate two relations between the known evaluation methods and ours. One relationship is that the fluctuation of measurement value and non-repeatability give an upper bound of the Monge distance. The other is, when the fluctuation of measurement value is zero, the diamond norm becomes well-defined and the value becomes the same as the non-repeatability.

We calculate a sufficient time to guarantee the fluctuation of measurement

value below some small value ε , for each of the two measurement schemes. We find that the tomography-based method takes the time proportional to $O(d^4 \Delta_{\max} / \varepsilon)$, while the phase estimation based method takes $O(\Delta_{\max}^3 / \varepsilon^2)$, where d is the dimension of the target system and Δ_{\max} is the difference between the largest energy eigenvalue and the smallest energy eigenvalue. It is clarified that when the fluctuation of measurement value is smaller than Δ_{\max}^2 / d^4 , the tomography-based method is better than the phase estimation based method. However, the dimension of a physical system grows exponentially with system size given by the number of constituent particles whereas Δ_{\max} grows only linearly when we assume a nearest-neighbor interaction between particles, which is frequently encountered in physics. Therefore, as for the fluctuation of measurement value, phase estimation based method shows better performance when the system size is sufficiently large. We also calculate the non-repeatability for the case of tomography-based method and the phase estimation algorithm based method. We have found the non-repeatability of the tomography-based method can not converge to zero in the limit of infinite measurement time, while that of the method using phase estimation algorithm is always zero for any amount of time consumed.

Chapter 2

Preliminaries

2.1 Introduction

In this chapter, we present a formulation of quantum mechanics used in quantum information theory. In Sec. 2.2, we give mathematical preliminaries. In Sec. 2.3, we present axioms of the theory of quantum mechanics. In Sec. 2.4 we present definitions and notations of terminologies of quantum measurement used in this thesis.

2.2 Mathematical Preliminary

A Hilbert space is a vector space associated with a distance in which all Cauchy sequences have a limit point (completeness). Concepts in quantum mechanics are defined on a Hilbert space. In this thesis, we only consider the Hilbert spaces of finite dimensions. In the following, we first set notations of general terms in the linear algebra used in the thesis. Second, we give definitions for mathematical terms to formulate quantum mechanics for mixed states.

Notations on finite dimensional Hilbert spaces

Notation 1. We call a finite dimensional complex vector space \mathbb{C}^d as a Hilbert space, and we represent it by a curly alphabet \mathcal{H} . We represent the inner product between two vectors $|\psi\rangle, |\phi\rangle \in \mathcal{H}$ as $\langle\phi|\psi\rangle$, and the norm of a vector $|\psi\rangle$ as $\| |\psi\rangle \| = \sqrt{\langle\psi|\psi\rangle}$.

Notation 2. We call a linear operator on \mathcal{H} simply as an operator. $\mathcal{B}(\mathcal{H})$ denotes the set of operators on \mathcal{H} . We represent the identity operator on \mathcal{H} as $I \in \mathcal{B}(\mathcal{H})$.

Notation 3. For a diagonalizable (normal) operator $A \in \mathcal{B}(\mathcal{H})$, we represent a projection operators corresponding to the eigenspace of the i -th eigenvalue a_i as P_i^A . Thus the operator A is written by

$$A = \sum_i a_i P_i^A. \quad (2.1)$$

Notation 4. We represent the tensor product of two vectors as $|\psi\rangle \otimes |\phi\rangle$ for vectors $|\psi\rangle \in \mathcal{H}$ and $|\phi\rangle \in \mathcal{H}'$ and also as $|\psi\rangle|\phi\rangle \in \mathcal{H} \otimes \mathcal{H}'$ for short.

Definitions on finite dimensional Hilbert spaces

Definition 1. An Hermitian operator whose eigenvalues are non-negative is called a positive matrix. For any Hermite operator $A \in \mathcal{B}(\mathcal{H})$, $A \geq 0$ means the Hermitian operator A is a positive matrix.

Definition 2. When $\rho \in \mathcal{B}(\mathcal{H})$ satisfies

$$\rho \geq 0, \quad \text{Tr}[\rho] = 1, \quad (2.2)$$

it is called as a density operator (matrix) on \mathcal{H} . $\mathcal{D}(\mathcal{H})$ denotes the set of density operators.

Definition 3. For $|\psi\rangle, |\phi\rangle \in \mathcal{H}$, an operator $|\xi\rangle\langle\phi| \in \mathcal{B}(\mathcal{H})$ is defined by,

$$(|\psi\rangle\langle\phi|)|\xi\rangle := \langle\phi|\xi\rangle \cdot |\psi\rangle. \quad (2.3)$$

Definition 4. For $A \in \mathcal{B}(\mathcal{H} \otimes \mathcal{H}')$ such that

$$A := \sum_{i,j} |e_i\rangle\langle e_j| \otimes A_{ij}, \quad |e_i\rangle \in \mathcal{H}, \quad A_{ij} \in \mathcal{B}(\mathcal{H}'), \quad (2.4)$$

we define a linear map $\text{Tr}_{\mathcal{H}'}[*] : \mathcal{B}(\mathcal{H} \otimes \mathcal{H}') \rightarrow \mathcal{B}(\mathcal{H})$, which is called the partial trace of A over \mathcal{H}' as

$$\text{Tr}_{\mathcal{H}'}[A] := \sum_{i,j} \text{Tr}[A_{ij}] |e_i\rangle\langle e_j|. \quad (2.5)$$

Definition 5. For any Hermite operator A on \mathcal{H} and real function $f : \mathbb{R} \rightarrow \mathbb{R}$, we define the Hermite operator $f(A)$ on \mathcal{H} by

$$f(A) = \sum_i f(a_i) P_i^A. \quad (2.6)$$

Definition 6. We define the trace-norm of an operator $A \in \mathcal{B}(\mathcal{H})$ as

$$\|A\|_{tr} := \text{Tr}[\sqrt{AA^\dagger}]. \quad (2.7)$$

Definition 7. A linear function $\mathcal{A} : \mathcal{B}(\mathcal{H}) \rightarrow \mathcal{B}(\mathcal{H})$ is called a superoperator on the Hilbert space \mathcal{H} . We represent the identity superoperator on \mathcal{H} as id and also as $\text{id}_{\mathcal{H}}$ to specify the Hilbert space. We represent superoperators by curly alphabets or Greek alphabets distinguishing them from operators on \mathcal{H} .

Definition 8. We define the tensor product of two superoperators Γ on \mathcal{H} and Λ on \mathcal{H}' as

$$(\Gamma \otimes \Lambda)A := \sum_{i,j} \Gamma(|e_i\rangle\langle e_j|) \otimes \Lambda(A_{ij}), \quad (2.8)$$

where $A \in \mathcal{B}(\mathcal{H} \otimes \mathcal{H}')$ is defined by

$$A := \sum_{i,j} |e_i\rangle\langle e_j| \otimes A_{ij}, \quad |e_i\rangle \in \mathcal{H}, \quad A_{ij} \in \mathcal{B}(\mathcal{H}'). \quad (2.9)$$

Definition 9. A superoperator Γ on \mathcal{H} is a completely positive (CP) map if and only if

$$A \geq 0 \Rightarrow \Gamma \otimes \text{id}_{\mathcal{H}'}(A) \geq 0, \quad (2.10)$$

is satisfied for all Hilbert spaces \mathcal{H}' and Hermite operators A on $\mathcal{H} \otimes \mathcal{H}'$.

Definition 10. A superoperator Γ on \mathcal{H} is a completely positive trace preserving (CPTP) map if and only if

$$A \geq 0 \Rightarrow \Gamma \otimes \text{id}_{\mathcal{H}'}(A) \geq 0, \quad (2.11)$$

$$\text{Tr}[A] = \text{Tr}[\Gamma(A)], \quad (2.12)$$

are satisfied for all Hilbert spaces \mathcal{H}' and operators $A \in \mathcal{B}(\mathcal{H} \otimes \mathcal{H}')$.

As the last part of this subsection, we introduce the following fact [36].

Fact 1. The partial trace and a tensor product of superoperators are defined independent of the chosen basis set.

2.3 Formalisms of quantum mechanics

We summarize two formalisms of quantum mechanics. One is the observable formalism for pure states introduced by von Neumann [6], and the other is the instrument formalism for mixed states widely used in quantum information. We present both formalisms based on the axioms of quantum mechanics for pure and mixed state. We will combine these two formalisms to develop an instrument formalism of measurement of observables in the next section.

The observable formalism for pure states

Axiom 1. Any quantum system corresponds to a Hilbert space \mathcal{H} . A state of a system is characterized by a unit vector $|\psi\rangle \in \mathcal{H}$.

Axiom 2. Any observable corresponds to an Hermitian operator $A \in \mathcal{B}(\mathcal{H})$. When an observable A is measured on a state $|\psi\rangle$, we obtain one of the eigenvalues of A as an outcome. The probability p_i of obtaining the eigenvalue a_i of A is given by

$$p_i = \langle \psi | P_i^A | \psi \rangle, \quad (2.13)$$

and the post-measurement state $|\psi_i\rangle$ after obtaining an eigenvalue a_i becomes

$$|\psi_i\rangle = \frac{P_i^A |\psi\rangle}{\|P_i^A |\psi\rangle\|}. \quad (2.14)$$

Axiom 3. For any quantum system represented by a Hilbert space \mathcal{H} , there is an Hermite operator $H \in \mathcal{B}(\mathcal{H})$ which is called the Hamiltonian of a system, such that the state $|\psi\rangle \in \mathcal{H}$ after time t is described as

$$|\psi(t)\rangle = e^{-iHt}|\psi\rangle, \quad (2.15)$$

when the system is closed.

Axiom 4. For two different quantum systems represented by \mathcal{H} and \mathcal{H}' , the total system is characterized by the Hilbert space $\mathcal{H} \otimes \mathcal{H}'$.

The instrument formalism for mixed states

In a standard textbook of quantum information theory [36], measurement outcomes are introduced as a list of *outcomes* (indices). This is because what we obtain by a measurement is not only a real-valued outcome but a *stochastic event* in general. For example, by a measurement inserting a polarizing plate into the path of a photon, one of the following two mutually exclusive events occurs, one event is that the photon is absorbed into the plate, and the other is that the photon passes through the plate. There is no real such as eigenvalues of observables obtained from this measurement, but assigning number 0 to the former event and 1 to the latter, we can distinguish each event by each *index*. In accordance with this generalized idea of quantum measurement, we describe outcomes of a measurement by a list of indices distinguishing stochastic events.

Axiom 5. Any quantum system corresponds to a Hilbert space \mathcal{H} . A state in a system is characterized by a density operator $\rho \in \mathcal{D}(\mathcal{H})$. An ensemble of states that where each state $\rho_i \in \mathcal{D}(\mathcal{H})$ appears in probability p_i is characterized as a state

$$\rho = \sum_i p_i \rho_i. \quad (2.16)$$

Axiom 6. A set of CP maps $\mathcal{I} = \{\mathcal{I}_i | i \in X\}$ on \mathcal{H} is called a measurement instrument if and only if the superoperator

$$\Lambda_{\mathcal{I}} = \sum_{i \in X} \mathcal{I}_i \quad (2.17)$$

becomes a CPTP map. Any measurement process corresponds to a measurement instrument (or an instrument for short) on \mathcal{H} . Each stochastic event of the measurement is represented as one of indices in X . When \mathcal{I} is measured on a state ρ , the probability p_i of obtaining the i -th event is

$$p_i := \text{Tr}[\mathcal{I}_i \rho], \quad (2.18)$$

and the post measurement state ρ_i after obtaining the event is

$$\rho_i = \frac{\mathcal{I}_i \rho}{\text{Tr}[\mathcal{I}_i \rho]}. \quad (2.19)$$

Axiom 7. For any quantum system, there is an Hermite operator $H \in \mathcal{B}(\mathcal{H})$ which is called the Hamiltonian, for an initial state $\rho \in \mathcal{D}(\mathcal{H})$, the state after duration time t is described by

$$\rho(t) = e^{-iHt} \rho e^{iHt}. \quad (2.20)$$

Energy is an observable on \mathcal{H} and it corresponds to the Hamiltonian of the system.

Axiom 8. For two different systems \mathcal{H} and \mathcal{H}' , the total system is characterized by the Hilbert space $\mathcal{H} \otimes \mathcal{H}'$. For a state $\rho_{\text{tot}} \in \mathcal{D}(\mathcal{H} \otimes \mathcal{H}')$ on the total system $\mathcal{H} \otimes \mathcal{H}'$, the state of the subsystem \mathcal{H} denoted is given by

$$\rho = \text{Tr}_{\mathcal{H}'} [\rho_{\text{tot}}]. \quad (2.21)$$

We call ρ as the reduced density operator (matrix) of ρ_{tot} on \mathcal{H} .

A state represented by $|\psi\rangle \in \mathcal{H}$ corresponds to the rank-1 projection operator $|\psi\rangle\langle\psi| \in \mathcal{D}(\mathcal{H})$ in the formalism for mixed state. States represented by rank-1 projective operators are called pure states. Other density operators in \mathcal{H} are called mixed states.

Note that the CPTP map $\Lambda_{\mathcal{I}}$ in Axiom 6 gives an averaged post-measurement state of the measurement \mathcal{I} on ρ , since

$$\Lambda_{\mathcal{I}} \rho = \sum_i p_i \rho_i. \quad (2.22)$$

It should be noted that the term *measurement* in the instrument formalism represents a wider scope of measurement than the one in the pure state formalism. An instrument including only one CP(TP) map (only one event happening independently of a given state) is also called a measurement, nevertheless no information of a state ρ is extracted. Even if there is no observer, when a state change $\rho \rightarrow \Lambda_i \rho$ characterized by a CPTP map Λ_i with a probability p_i , we could describe this process as a measurement instrument $\mathcal{I} = \{p_i \Lambda_i | i \in X\}$. That is, any stochastic state change obtaining from non-closedness of a quantum system is characterized by an instrument.

2.4 Measurement in quantum mechanics

In the instrument formalism, measurements are not necessary to correspond to Hermite operators. Moreover, measurement in the instrument formalism does not give real-valued outcomes, but just indices of events. In this thesis, we construct a quantum measurement described in the instrument formalism to simulate the measurement of an observable, energy. To do this, we need to associate a real-value outcome to each event of an instrument. Thus we formulate the following definition of measurements.

Definition 11. *We define a real valued function $x : X \rightarrow \mathbb{R}$ which associates the i -th event to a real number x_i . We call x as an measurement value. We call the combination of measurement instrument and a measurement outcome as a measurement value, and denote it as $\mathcal{M} = \{\mathcal{I}, x, X\}$.*

The instrument of a measurement corresponds to the substantial measurement procedure, but it does not provide the correspondence between the index of the event i and the real valued measurement value x_i . The function, x is the part of bridging the index and the real valued measurement value. For example, in Stern-Gerlach's experiment, applying the magnetic field on a spin particle and the detection of the position of the particle correspond to the measurement instrument. Finding out the spin particle in a position (upper half/lower half) is an event of this measurement. We calculate the spin from the position of the particle; this process is described by the function of measurement value.

According to this definition of measurement, we also formulate probability measure of outcomes.

Definition 12. *For a measurement $\mathcal{M} = \{\mathcal{I}, x, X\}$, we define a map $\mu^{\mathcal{M}}$ from a density matrix ρ to probability measure*

$$\mu_{\rho}^{\mathcal{M}}(B) = \sum_{i \in a^{-1}(B)} \text{Tr}[\mathcal{I}_i \rho], \quad (2.23)$$

where $B \subset \mathbb{R}$.

Note that this measure does not reflect the property of the state change by a measurement; thus the map from \mathcal{M} to $\mu_{\rho}^{\mathcal{M}}$ is not an injection.

Definition 13. *For any real function $f : \mathbb{R} \rightarrow \mathbb{R}$, we define the expectation value of f under the probability measure μ as*

$$\langle f \rangle_{\mu} := \int \mu_{\rho}(dx) f(x). \quad (2.24)$$

We also define the following superoperator on the Hilbert space \mathcal{H}

$$\mathcal{I}(f) := \sum_i f(x_i) \mathcal{I}_i. \quad (2.25)$$

We define the expectation value of f in μ_ρ^M as

$$\langle f \rangle_{\mu_\rho^M} := \text{Tr}[\mathcal{I}(f)\rho]. \quad (2.26)$$

By using these definitions, we can represent the measurements corresponding instrument formalism of observables for mixed states. We call this type of measurements as the projective measurement.

Definition 14. Consider that a Hilbert space \mathcal{H} is composed by mutually orthogonal subspaces \mathcal{H}_i as $\mathcal{H} = \bigoplus_{i \in X} \mathcal{H}_i$. By using a projector P_i onto the subspace \mathcal{H}_i , we define the following projective superoperator $\mathcal{P}_i \in \mathcal{B}(\mathcal{H})$ as

$$\mathcal{P}_i \rho = P_i \rho P_i. \quad (2.27)$$

We call $\mathcal{P} = \{\mathcal{P}_i | i \in X\}$ as projective measurement instruments. We also call $\{\mathcal{P}, a, X\}$ as the projective measurement. For each projective measurement, we can define a unique Hermitian operator $A = \sum_i a_i P_i$ an observable. We denote \mathcal{M}^A as $\{\mathcal{P}, a, X\}$ and μ_ρ^A as the probability measure associated to this measurement. The expectation value of the observable A in a quantum state ρ is given by

$$\langle A \rangle_\rho = \langle 1 \rangle_{\mu_\rho^A} = \text{Tr}[A\rho]. \quad (2.28)$$

If the observable of a projective measurement is the Hamiltonian H of the quantum system, the measurement is called projective measurement of energy.

Chapter 3

Performance of the measurement

3.1 Introduction

Apart from von Neumann's original axiom of quantum mechanics [6] (the measurement in observable formalism for pure state), today the word *measurement* refers to different operations depending on the field of physics. Each field of quantum physics has developed its own notation of measurement. For condensed matter physicists or the others interested in macroscopic behaviors in quantum systems, the expectation value $\langle \psi | A | \psi \rangle$ is the quantities of interest on measurement. On the other hand, for quantum information scientists or other physicists who are interested in manipulation of microscopic quantum states, the probabilities of possible events and state changes associated with them are the most interesting properties on measurement, since they apply these properties for computation and readout. For them, the measurement values are only identifiers for discriminating events; then each of them is described just as an index i instead of the real number a_i . By these differences on what they required for measurements, various evaluations of the performance of a measurement has been proposed before.

Our goal is to formulate a method of evaluating how a measurement is close to (far from) an ideal projective measurement. In this chapter, we first introduce previously known two evaluations of the performance of a measurement in Sec. 3.2. One is the Monge distance, the distance between two probability distributions. The other is the diamond norm, the distance between two measurement instruments. Unfortunately, these two evaluations are not applicable for our goal. Thus, we introduce two new evaluation methods, *fluctuation of measurement value* and *non-repeatability* in Sec. 3.3. In this same section, we formulate two relations between the known evaluation methods and ours. One relationship is that the fluctuation of measurement value and non-repeatability give an upper bound of the Monge distance. The other is, when the fluctuation of measurement value is zero, the diamond norm becomes well-defined and the value becomes the same as the non-repeatability.

3.2 Previously known evaluation of performance

3.2.1 Evaluation as a probability distribution; Monge distance

The Monge distance is originally proposed in the optimal transport problem of soil redistribution problem in a construction site [27, 28]. The essence of this problem is captured in the following way. There is an amount of soil piled in a shape on the ground and we want to redistribute the soil the soil piled in the

different shape while preserving the total amount of the soil. What is the optimal way to transport when the cost of the transport is given by the total migration length of all the particles of the soil. We represent the distributions of the soil before and after the transportation by probability measures by taking normalization for the distributions. Consider a distribution of the soil on the ground given by a probability measure μ on an Euclidian space \mathbb{R}^n , and transfer the soil at $x \in \mathbb{R}^n$ to $y \in \mathbb{R}^n$. The function $\Phi(x) := y$ representing a way of transportation must satisfy that $\nu(B) := \mu(\Phi^{-1}(B))$, where ν is the distribution of the soil after the transportation. The cost $c(\Phi)$ to be minimized in the optimal transport problem is given as

$$c(\Phi) = \int_{\mathbb{R}^n} d\mu(x) \|x - \Phi(x)\|, \quad (3.1)$$

where $\|\cdot\|$ is the Euclidean norm. A major progress on solving the optimal transport problem was made by Kantorovich in 1940's. On the way for solving another optimization problem, it was found that the optimal transport problem is equivalent to a dual problem [29, 28] to find a function $f \in L$ which maximize the following value $C(f)$

$$C(f) = |\langle f \rangle_\mu - \langle f \rangle_\nu|, \quad \langle f \rangle_\mu = \int_{\mathbb{R}^n} d\mu(x) f(x), \quad \langle f \rangle_\nu = \int_{\mathbb{R}^n} d\nu(x) f(x), \quad (3.2)$$

where

$$L = \left\{ f : \mathbb{R} \rightarrow \mathbb{R} \mid |f(x) - f(y)| \leq \|x - y\| \right\}. \quad (3.3)$$

The supremum of $C(f)$ is equal to the infimum of $c(\Phi)$. This relationship is known as *Monge-Kantorovich duality*. In this thesis we define the distance between two probability measures as the supremum value of $C(f)$.

Definition 15. *Monge distance $\|\cdot\|_m$ between two measures μ, ν is defined as*

$$\|\mu - \nu\|_m := \sup_{f \in L} |\langle f \rangle_\mu - \langle f \rangle_\nu|. \quad (3.4)$$

where

$$L := \left\{ f : \mathbb{R} \rightarrow \mathbb{R} \mid |f(x) - f(y)| \leq \|x - y\| \right\}. \quad (3.5)$$

We call $f \in L$ as a *Lipschitz function*.

In the study of quantum physics, the Monge distance has been used for evaluating the distance between two measurements. In a study of an uncertainty relationship [30], this distance is regarded as an error of a measurement simulating an ideal measurement of an observable.

Definition 16. We define the Monge distance between two measurements $\mathcal{M} = \{I, a, X\}$ and $\mathcal{M}' = \{I', a', X'\}$ on a Hilbert space \mathcal{H} as

$$\|\mathcal{M} - \mathcal{M}'\|_m := \sup_{\rho \in D(\mathcal{H})} \|\mu_\rho^{\mathcal{M}} - \mu_\rho^{\mathcal{M}'}\|_m, \quad (3.6)$$

Other methods for evaluating an error of a measurement from the ideal measurement, for example the one defined by Arthurs and Goodman [31], focus on the error appearing in the expectation values of an observable. They evaluate how the measurement values are different from the expectation value of an observable. In this type of method, error can be small when the measurement values are close to the expectation value although the probability distribution of the measurement values are totally different. In contrast, the Monge distance evaluates the distance of the measurement as the distance between probability distributions.

The Monge distance between a projective measurement \mathcal{M}^A of an observable A and its simulation \mathcal{M} gives the upper bound of the difference in expectation values whose measurement value is deformed by a Lipschitz function f

$$\forall f \in L, \forall \rho \in D(\mathcal{H}), \quad \left| \langle f(A) \rangle_\rho - \langle f \rangle_{\mu_\rho^{\mathcal{M}}} \right| \leq \|\mathcal{M}^A - \mathcal{M}\|_m. \quad (3.7)$$

Among distances between two probability distributions, the Monge distance is particularly suitable to evaluate the distance between two Dirac distributions due to the following reasons. Let us define a Dirac measure μ_x for a real number $x \in \mathbb{R}$ which satisfies $\mu_x(B) = 1$ when $x \in B$, while $\mu_x(B) = 0$ otherwise. Consider there are two probability measures μ_0 and μ_ε representing two different measurements on the same state, where $\varepsilon > 0$. The measurement according to μ_0 always returns the measurement value 0, otherwise the one of μ_ε returns ε . Intuitively, the closer the value ε is to zero, the better the performance the measurement μ_ε shows as a simulation of μ_0 . However, some distances of measure do not behave like this intuition. For example, consider the total variance measure for a bounded measure μ on the real numbers defined as

$$|\mu|(B) := \sup_{C \in \mathcal{B}(B)} \mu(C) - \inf_{C \in \mathcal{B}(B)} \mu(C), \quad (3.8)$$

where $\mathcal{B}(B)$ is the subset of the Borel set included in $B \subset \mathbb{R}$. By using this measure, we can introduce a distance between two bounded measures μ, ν on real numbers as

$$\|\mu - \nu\|_1 := |\mu - \nu|(\mathbb{R}), \quad (3.9)$$

which corresponds to the L^1 distance between two functions. Because there is always an element C of the Borel set which can separate $\varepsilon \in \mathbb{R}$ from $0 \in \mathbb{R}$, for example a radius ε open ball centered at 0, we have

$$\|\mu_0 - \mu_\varepsilon\|_1 = 2. \quad (3.10)$$

Thus ε is not taken into account for this quantity.

Since a quantum measurement in the finite dimensional Hilbert space has a discrete probability distribution, the probability distribution of measurement values can be decomposed into a convex combination of the Dirac measures. For two discrete probability distributions μ, ν , the distance evaluated by the total variance is less than the maximum value 2 only when at least one of the common Dirac measures is included in both of the convex decompositions of μ and ν . However, such a combination of two probability measures is in the zero set in the parameter space. Therefore such a distance is not useful for our problem. The other way of evaluation in terms of relative entropy, has the same problem. On the other hand, since the amount of change of Lipschitz functions in ε -width is equal to or less than ε , the Monge distance between μ_0 and μ_ε is calculated as

$$\|\mu_0 - \mu_\varepsilon\|_m = \varepsilon. \quad (3.11)$$

The Monge distance reflects the metric of measurement values. Thus this distance is suitable for our problem.

3.2.2 Evaluation of state change; Diamond norm

When our interest is focused on the quantum state change caused by a measurement, the diamond norm [32, 33] is widely used in quantum information.

Definition 17. *If there are two measurement instruments $\mathcal{I} = \{\mathcal{I}_i | i \in X\}$ and $\mathcal{I}' = \{\mathcal{I}'_i | i \in X\}$ on a Hilbert space \mathcal{H} , the distance between two sets of measurement instruments measured by the diamond norm is given as*

$$D_\diamond(\mathcal{I}, \mathcal{I}') := \sum_{i \in X} \|\mathcal{I}'_i - \mathcal{I}_i\|_\diamond, \quad (3.12)$$

where $\|\cdot\|_\diamond$ is the diamond norm defined for any superoperator Λ on Hilbert space \mathcal{H} as

$$\|\Lambda\|_\diamond := \|\Lambda \otimes \text{id}_{\mathcal{H}}\|_{op} = \sup_{A \in \mathcal{B}(\mathcal{H} \otimes \mathcal{H})} \frac{\|(\Lambda \otimes \text{id}_{\mathcal{H}}) A\|_{\text{tr}}}{\|A\|_{\text{tr}}}. \quad (3.13)$$

$\mathcal{B}(\mathcal{H})$ is the set of matrices on \mathcal{H} , and the norm $\|\cdot\|_{\text{tr}}$ is defined as

$$\|A\|_{\text{tr}} := \text{Tr} \left[\sqrt{AA^\dagger} \right]. \quad (3.14)$$

This norm is often used to evaluate the difference between two CPTP maps in quantum information. An important operational meaning of the diamond norm is that two quantum state transformation represented by CPTP maps Λ, Λ' can be discriminated with success probability $1/2 + \|\Lambda - \Lambda'\|_\diamond / 4$ (Holmström's theorem).

For a superoperator Λ on a Hilbert space \mathcal{H} , its effect on a larger system $\mathcal{H} \otimes \mathcal{H}'$ can be larger in the operator norm than the that of on \mathcal{H} as

$$\|\Gamma\|_{op} \leq \|\Gamma \otimes \text{id}_{\mathcal{H}'}\|_{op}. \quad (3.15)$$

The diamond norm is proposed for giving the upper bound of the operator norm over all the extended Hilbert spaces. The maximum operator norm is achieved when the extended Hilbert space is $\mathcal{H}^{\otimes 2}$ [34], namely

$$\|\Gamma \otimes \text{id}_{\mathcal{H}'}\|_{op} \leq \|\Gamma \otimes \text{id}_{\mathcal{H}}\|_{op} = \|\Gamma \otimes \text{id}_{\mathcal{H}''}\|_{op}, \quad (3.16)$$

$$\dim \mathcal{H}' \leq \dim \mathcal{H} \leq \dim \mathcal{H}'' . \quad (3.17)$$

Thus it is enough to consider $\|\Gamma \otimes \text{id}_{\mathcal{H}}\|_{op}$ to find the bound. For this reason, the diamond norm $\|\cdot\|_{\diamond}$ of a superoperator \mathcal{S} on the Hilbert space \mathcal{H} can be calculated as

$$\|\Gamma\|_{\diamond} = \|\Gamma \otimes \text{id}_{\mathcal{H}}\|_{op}. \quad (3.18)$$

The following lemma is convenient for calculating the diamond norm [34].

Lemma 1. *For any Hermitian preserving superoperator Γ on the Hilbert space \mathcal{H} ,*

$$\|\Gamma\|_{\diamond} = \max_{P \in \mathcal{P}_1(\mathcal{H} \otimes \mathcal{H})} \|(\Gamma \otimes \text{id}_{\mathcal{H}}) P\|_{\text{tr}}, \quad (3.19)$$

where $\mathcal{P}_1(\mathcal{H} \otimes \mathcal{H})$ is a set of rank-1 projectors on $\mathcal{H}^{\otimes 2}$ is satisfied.

By definition, this distance is determined only for two measurements sharing a common set of indices X . If it is not the case, a coarse graining method is proposed for adjusting the numbers of indices.

Definition 18. *Consider there is a measurement instrument $\mathcal{I} = \{\mathcal{I}_i | i \in X\}$. A coarse-grained measurement instrument $\tilde{\mathcal{I}} = \{\tilde{\mathcal{I}}_{X_i} | i \in Y\}$ such that*

$$\tilde{\mathcal{I}}_{X_i} = \sum_{k \in X_i} \mathcal{I}_k. \quad (3.20)$$

is defined for disjoint subsets $X_i \subset X$ satisfying $\bigcup_{i \in Y} X_i = X$.

The coarse graining is not only used for reducing the number of CP-maps but also for increasing the number by adding empty sets as the disjoint sets.

To evaluate how the state changes due to two measurements $\mathcal{M}, \mathcal{M}'$ are close to each other, we define the following coarse graining.

Definition 19. Consider there are two measurements $\mathcal{M} = \{\mathcal{I}, x, X\}$ and $\mathcal{M}' = \{\mathcal{I}', x', X'\}$. For a countable disjoint cover C of \mathbb{R} such that

$$C := \left\{ c_i \subset \mathbb{R} \mid i \neq j, c_i \cap c_j = \emptyset, \bigcup_i c_i = \mathbb{R}, \right\}, \quad (3.21)$$

we define coarse-grained measurement instruments for C as

$$\tilde{\mathcal{I}}_C = \{\tilde{\mathcal{I}}_{x^{-1}c_i} \mid i \in \mathbb{Z}\}, \quad \tilde{\mathcal{I}}'_C = \{\tilde{\mathcal{I}}'_{x'^{-1}c_i} \mid i \in \mathbb{Z}\}. \quad (3.22)$$

The diamond norm between these two measurement instruments is defined by

$$D_\diamond(\tilde{\mathcal{I}}_C, \tilde{\mathcal{I}}'_C) := \sum_{i \in \mathbb{Z}} \left\| \tilde{\mathcal{I}}_{x^{-1}c_i} - \tilde{\mathcal{I}}'_{x'^{-1}c_i} \right\|_\diamond \quad (3.23)$$

Note that this distance is not uniquely determined for \mathcal{M} and \mathcal{M}' because it depends on the countable disjoint cover C of \mathbb{R} .

By using the triangular inequality, the following lemma is derived naturally.

Lemma 2. When two countable disjoint covers of \mathbb{R} given by

$$C = \left\{ c_i \subset \mathbb{R} \mid i \neq j, c_i \cap c_j = \emptyset, \bigcup_i c_i = \mathbb{R}, \right\}, \quad (3.24)$$

and

$$C' = \left\{ c'_i \subset \mathbb{R} \mid i \neq j, c'_i \cap c'_j = \emptyset, \bigcup_i c'_i = \mathbb{R}, \right\}. \quad (3.25)$$

satisfy

$$C \leq C' \stackrel{\text{def}}{\iff} \forall i, \exists j, c_i \subset c'_j, \quad (3.26)$$

then

$$D_\diamond(\tilde{\mathcal{I}}_{C'}, \tilde{\mathcal{I}}'_{C'}) \leq D_\diamond(\tilde{\mathcal{I}}_C, \tilde{\mathcal{I}}'_C). \quad (3.27)$$

The semiordering between families of subsets of \mathbb{R} in Lemma 2 represents the comparison on the coarse-grainedness. As a distance between two measurements independent of C , we introduce the following a fine-grained limit of the diamond norm between two measurement instruments.

Definition 20. Consider there are two measurements $\mathcal{M} = \{\mathcal{I}, x, X\}$ and $\mathcal{M}' = \{\mathcal{I}', x', X'\}$. We define the fine-grained limit of the diamond norm.

$$D_\diamond(\mathcal{M}, \mathcal{M}') = \max_{C \in \mathcal{C}(\mathbb{R})} D_\diamond(\tilde{\mathcal{I}}_C, \tilde{\mathcal{I}}'_C), \quad (3.28)$$

where $\mathcal{C}(\mathbb{R})$ is a set of countable disjoint cover of \mathbb{R} .

The fine grained limit of the diamond norm is well-defined. The following theorem guarantees the well-definedness.

Theorem 1. *Consider there are two measurements $\mathcal{M} = \{\mathcal{I}, x, X\}$ and $\mathcal{M}' = \{\mathcal{I}', x', X'\}$. The fine-grained limit of the diamond norm $D_\diamond(\mathcal{M}, \mathcal{M}')$ exists and the value is given by*

$$D_\diamond(\mathcal{M}, \mathcal{M}') = \sum_{a \in \text{Im}x \setminus \text{Im}x'} \|\tilde{\mathcal{I}}_{x^{-1}a}\|_\diamond + \sum_{a \in \text{Im}x' \setminus \text{Im}x} \|\tilde{\mathcal{I}}'_{x'^{-1}a}\|_\diamond + \sum_{a \in \text{Im}x' \cap \text{Im}x} \|\tilde{\mathcal{I}}_{x^{-1}a} - \tilde{\mathcal{I}}'_{x'^{-1}a}\|_\diamond. \quad (3.29)$$

Proof. Let us define the following countable disjoint cover C_0 of \mathbb{R} .

$$C_0 := \{\{a\} \mid a \in \text{Im}x \cup \text{Im}x'\} \cup \{\mathbb{R} \setminus (\text{Im}x \cup \text{Im}x')\}. \quad (3.30)$$

We also define the intersection of two countable disjoint covers of \mathbb{R} as

$$C \cap C' = \{c_i \cap c'_j \mid c_i \in C, c'_j \in C'\} \quad (3.31)$$

By definition, $C \cap C'$ satisfies $C \cap C' \leq C$.

For any $c_i \in C$, one of the following two cases are satisfied for a measurement $\mathcal{M} = \{\mathcal{I}, x, X\}$.

$$\exists k \in X, \quad x_k \in c_i, \quad \text{or} \quad x^{-1}c_i = \emptyset. \quad (3.32)$$

In the former case

$$\tilde{\mathcal{I}}_{x^{-1}c_i} = \sum_{k \in x^{-1}c_i} \mathcal{I}_k, \quad (3.33)$$

and in the latter case

$$\tilde{\mathcal{I}}_{x^{-1}c_i} = 0. \quad (3.34)$$

Therefore we derive

$$\begin{aligned} \left\| \tilde{\mathcal{I}}_{x^{-1}c_i} - \tilde{\mathcal{I}}'_{x'^{-1}c_i} \right\|_\diamond &= \left\| \tilde{\mathcal{I}}_{x^{-1}c_i} - \tilde{\mathcal{I}}'_{x'^{-1}c_i} \right\|_\diamond \quad (x^{-1}c_i \subset \text{Im}x \cap \text{Im}x'), \\ &= \left\| \tilde{\mathcal{I}}_{x^{-1}c_i} \right\|_\diamond \quad (x^{-1}c_i \subset \text{Im}x \setminus \text{Im}x'), \\ &= \left\| \tilde{\mathcal{I}}'_{x'^{-1}c_i} \right\|_\diamond \quad (x^{-1}c_i \subset \text{Im}x' \setminus \text{Im}x), \\ &= 0 \quad (c_i \cap (\text{Im}x \cup \text{Im}x') = \emptyset). \end{aligned} \quad (3.35)$$

Let us consider the countable disjoint cover C is given by $C = C' \cap C_0$ where C' is another countable disjoint cover of \mathbb{R} . In this case, since all c_i including at least

one element of $\text{Im}x \cup \text{Im}x'$ must be a one-point set, Eq. (3.35) is represented by

$$\begin{aligned}
\left\| \tilde{\mathcal{I}}_{x^{-1}c_i} - \tilde{\mathcal{I}}'_{x'^{-1}c_i} \right\|_{\diamond} &= \left\| \tilde{\mathcal{I}}_{x^{-1}a} - \tilde{\mathcal{I}}'_{x'^{-1}a} \right\|_{\diamond} \quad (\exists^1 a \in \text{Im}x \cup \text{Im}x', a \in c_i), \\
&= \left\| \tilde{\mathcal{I}}_{x^{-1}a} \right\|_{\diamond} \quad (\exists^1 a \in \text{Im}x \setminus \text{Im}x', a \in c_i), \\
&= \left\| \tilde{\mathcal{I}}'_{x'^{-1}a} \right\|_{\diamond} \quad (\exists^1 a \in \text{Im}x' \setminus \text{Im}x, a \in c_i), \\
&= 0 \quad (\forall a \in \text{Im}x \cup \text{Im}x', a \notin c_i). \tag{3.36}
\end{aligned}$$

Thus the right hand side of Eq. (3.29) is achievable when $C = C' \cap C_0$. On the other hand, let we define a sequence of countable disjoint covers $C_k \in \mathcal{C}(\mathbb{R})$ satisfying

$$\lim_{k \rightarrow \infty} D_{\diamond}(\tilde{\mathcal{I}}_{C_k} - \tilde{\mathcal{I}}'_{C_k}) = \sup_{C \in \mathcal{C}(\mathbb{R})} D_{\diamond}(\tilde{\mathcal{I}}_C - \tilde{\mathcal{I}}'_C). \tag{3.37}$$

Because of Lemma 2, $C_k \cap C_0$ is also a sequence of countable disjoint covers approaching to the supremum. Then we have

$$\begin{aligned}
\sup_{C \in \mathcal{C}(\mathbb{R})} D_{\diamond}(\tilde{\mathcal{I}}_C - \tilde{\mathcal{I}}'_C) &= \lim_{k \rightarrow \infty} D_{\diamond}(\tilde{\mathcal{I}}_{C_k \cap C_0} - \tilde{\mathcal{I}}'_{C_k \cap C_0}) \\
&= \sum_{a \in \text{Im}x \setminus \text{Im}x'} \left\| \tilde{\mathcal{I}}_{x^{-1}a} \right\|_{\diamond} + \sum_{a \in \text{Im}x' \setminus \text{Im}x} \left\| \tilde{\mathcal{I}}'_{x'^{-1}a} \right\|_{\diamond} + \sum_{a \in \text{Im}x' \cap \text{Im}x} \left\| \tilde{\mathcal{I}}_{x^{-1}a} - \tilde{\mathcal{I}}'_{x'^{-1}a} \right\|_{\diamond}. \tag{3.38}
\end{aligned}$$

Therefore the theorem is proven. \square

3.3 Performance of a measurement as the projective measurement

3.3.1 Fluctuation of the measurement value and non-repeatability

Note that neither the diamond norm nor the Monge distance take account of all the properties of measurements. The diamond norm gives a metric among measurement instruments, which is not considering measurement values required in a measurement. If we only use the diamond norm for evaluating the distances between measurements, we cannot avoid ambiguity originating from determining one choice from coarse-graining methods. Conversely the Monge distance is for the measurement values, and it does not take account of state changes caused by the measurements. Furthermore, the Monge distance is very hard to calculate since the calculation includes maximization over Lipschitz functions.

In the followings, we formulate two new quantities R_1 and R_2 , which evaluate how different a measurement is from a projective measurement of an observable A . These quantities are relatively easy to calculate, their meanings are intuitively

clear and they have useful relationships with the diamond norm and Monge distance. Before introducing these two values, let us denote the following notation of the decomposition of an observable A on a Hilbert space \mathcal{H} which we use throughout the following discussions,

$$A = \sum_{i \in Y} X_i P_i, \quad P_i^A = \sum_{\Gamma \in Z_i} |a_i^\lambda\rangle\langle a_i^\lambda|, \quad (3.39)$$

where $\{|a_i^\lambda\rangle | i \in Y, \lambda \in Z_i\}$ is an orthonormal basis of \mathcal{H} . Y is a set of indices which specify an eigenspace of an observable A and Z_i is a set of indices identifying a basis of a degenerated eigenspace corresponding to eigenvalue a_i .

Definition 21. For a measurement $\mathcal{M} = \{x, \mathcal{I}, X\}$, we define R_1 as

$$R_1(\mathcal{M}|A) := \max_{\substack{\{|a_i^\lambda\rangle\} \\ i \in Y, \lambda \in Z_i}} \sum_{j \in X} \text{Tr} \left[\mathcal{I}_j(|a_i^\lambda\rangle\langle a_i^\lambda|) \right] (a_i - x_j)^2, \quad (3.40)$$

where the maximization under $\{|a_i^\lambda\rangle\}$ means that the orthonormal basis of the degenerated space is determined as it achieves the maximum value. We also define R_2 as

$$R_2(\mathcal{M}|A) = \sum_{i \in Y} \max_{\substack{\{|a_i^\lambda\rangle\} \\ \lambda \in Z_i}} \left\| \Lambda_{\mathcal{I}}(|a_i^\lambda\rangle\langle a_i^\lambda|) - |a_i^\lambda\rangle\langle a_i^\lambda| \right\|_{\text{tr}}. \quad (3.41)$$

We call R_1 as fluctuation of the measurement value, and R_2 as non-repeatability of a measurement.

The behaviors of projective measurement reflected to R_1 and R_2 are summarized by the followings. 1. When an eigenstate of an observable A is prepared, the measurement value of the observable A is always identical to the eigenvalue. 2. When an eigenstate is prepared, the state after the measurement is unchanged and stays in the same eigenstate. These two quantities are similar to the ideas of the error and disturbance proposed to introduce Ozawa's inequality [26].

3.3.2 Relationship between Monge distance and diamond norm

The two quantities of projectiveness we have introduced in the previous subsection is related to the diamond norm and the Monge distance through the following two theorems.

Theorem 2. Let us define a measurement $\mathcal{M} = \{x, \mathcal{I}, X\}$ and an observable A on a Hilbert space \mathcal{H} . We denote the set of eigenvalues of A as $\{X_i | i \in Y\}$ and the

projective superoperator of the eigenspace as \mathcal{P}_i^A . The projective measurement of A is defined as

$$\mathcal{M}^A = \{\mathcal{P}^A, a, Y\}, \quad \mathcal{P}^A = \{\mathcal{P}_i^A | i \in Y\}, \quad \mathcal{P}_i^A \rho = P_i^A \rho P_i^A. \quad (3.42)$$

We denote disjoint subsets $\{X_i \subset X | i \in Y\}$ as

$$X_i = x^{-1} a_i \quad (3.43)$$

for every eigenvalue a_i of A . We also denote X_0 which includes all the indices which are not included in any X_i , namely

$$X_0 = \bigcap_{i \in Y} X \setminus X_i. \quad (3.44)$$

We define the following coarse-grained measurement instruments.

$$\tilde{\mathcal{I}} = \{\tilde{\mathcal{I}}_{X_i} | i \in Y \cup \{0\}\}, \quad \tilde{\mathcal{P}}^A = \{\mathcal{P}_i^A | i \in Y \cup \{0\}\}, \quad (3.45)$$

where $\mathcal{P}_0 = 0$. We also define the measurement instrument and measurement which are the extensions of \mathcal{I} and \mathcal{M} into the Hilbert space $\mathcal{H}^{\otimes 2}$ by

$$\mathcal{I} \otimes \text{id}_{\mathcal{H}} := \{\mathcal{I}_i \otimes \text{id}_{\mathcal{H}} | i \in X\}, \quad \mathcal{M} \otimes \text{id}_{\mathcal{H}} := \{x, \mathcal{I} \otimes \text{id}_{\mathcal{H}}, X\}. \quad (3.46)$$

If $R_1(\mathcal{M}|A) = 0$, then

$$R_2(\mathcal{M} \otimes \text{id}_{\mathcal{H}} | A \otimes I_{\mathcal{H}}) = D_{\diamond}(\tilde{\mathcal{I}}, \tilde{\mathcal{P}}) = D_{\diamond}(\mathcal{M}, \mathcal{M}^A). \quad (3.47)$$

In case the observable A has no degeneracy, if $R_1(\mathcal{M}|A)$, then

$$R_2(\mathcal{M}|A) = D_{\diamond}(\tilde{\mathcal{I}}, \tilde{\mathcal{P}}) = D_{\diamond}(\mathcal{M}, \mathcal{M}^A). \quad (3.48)$$

As we will see in the proof below, when $R_1 = 0$, each measurement value x_i of a measurement \mathcal{M} is equal to one of the eigenvalues of A ; otherwise the probability of achieving the measurement value is zero. The distance between the coarse-grained measurement instruments $D_{\diamond}(\tilde{\mathcal{I}}, \tilde{\mathcal{P}}^A)$ defined in Theorem 2 equals the summation of each diamond distance between measurement instruments \mathcal{I}_{X_i} and \mathcal{P}_i^A , both of which represent the state changes due to \mathcal{M} and \mathcal{M}^A after achieving an measurement value a_i .

Theorem 2 concludes the following corollary.

Corollary 1. $\mathcal{M} = \{x, \mathcal{I}, X\}$ satisfies $R_1(\mathcal{M}|A) = 0$ and $R_2(\mathcal{M} \otimes \text{id}_{\mathcal{H}} | A \otimes I_{\mathcal{H}}) = 0$, if and only if the coarse-grained measurement \mathcal{M} is equivalent to the projective measurement of an observable A as

$$\tilde{\mathcal{M}} = \tilde{\mathcal{M}}^A, \quad (3.49)$$

where

$$\tilde{\mathcal{M}} = \{a, \tilde{\mathcal{I}}, Y \cup \{0\}\}, \quad \tilde{\mathcal{M}}^A = \{a, \mathcal{P}, Y \cup \{0\}\}. \quad (3.50)$$

The other theorem is for the Monge distance. We can bound the Monge distance between two measurement from above by using R_1 and R_2 .

Theorem 3. *There is a bound of the Monge distance between a measurement \mathcal{M} and a projective measurement \mathcal{M}^A which is determined by $R_1(\mathcal{M}|A)$ and $R_2(\mathcal{M}|A)$ as*

$$\|\mathcal{M} - \mathcal{M}^A\|_m \leq 2\sqrt{R_1(\mathcal{M}|A)} + d\Delta x_{\max} \left(\sqrt{2R_2(\mathcal{M}, A)} + \frac{R_2(\mathcal{M}, A)}{2} \right), \quad (3.51)$$

where Δx_{\max} is the difference between the maximum and minimum measurement values of the measurement \mathcal{M} .

First, we prove Theorem 2. We prove this theorem according to the following two lemmas.

Lemma 3. *A measurement $\mathcal{M} = \{\mathcal{I}, x, X\}$ satisfies $R_1(\mathcal{M}|A) = 0$, if and only if*

$$\text{Tr} \left[\mathcal{I}_j (|a_i^\lambda\rangle\langle a_i^\lambda|) \right] \neq 0 \Rightarrow x_j = X_i \quad (3.52)$$

is satisfied for any choice of eigenbasis $\{|a_i^\lambda\rangle | i \in Y, \lambda \in Z\}$, where $|a_i^\lambda\rangle$ is an eigenstate of A of corresponding to eigenvalue a_i .

Proof. By definition of R_1 , if

$$\text{Tr} \left[\mathcal{I}_j (|a_i^\lambda\rangle\langle a_i^\lambda|) \right] (x_j - a_i)^2 = 0, \quad (3.53)$$

for all $i \in Y, \lambda \in Z, j \in X$ and the choice of eigenbasis $\{|a_i^\lambda\rangle\}$, then the fluctuation of measurement value satisfies $R_1(\mathcal{M}|A) = 0$. Thus the backward implication of Lemma 3 is satisfied. Next we prove the forward implication by its contraposition. When at least one of the $\text{Tr} \left[\mathcal{I}_j (|a_i^\lambda\rangle\langle a_i^\lambda|) \right] (x_j - a_i)^2$ becomes nonzero, then $R_1(\mathcal{M}, A)$ never becomes 0. Therefore the forward implication is also proven. \square

Lemma 4. *If a measurement $\mathcal{M} = \{\mathcal{I}, x, X\}$ satisfies $R_1(\mathcal{M}|A) = 0$, then for all eigenstates $|a_i^\lambda\rangle$ in the different eigenspaces of the observable A ,*

$$\mathcal{I}_j (|a_i^\lambda\rangle\langle a_j^\mu|) = 0. \quad (3.54)$$

Proof. To prove Lemma 4, we define two density matrices ρ_+ and ρ_-

$$\rho_+ = (s|a_i^\lambda\rangle + c|a_j^\mu\rangle) (s\langle a_i^\lambda| + c^*\langle a_j^\mu|), \quad (3.55)$$

$$\rho_- = (s|a_i^\lambda\rangle - c|a_j^\mu\rangle) (s\langle a_i^\lambda| - c^*\langle a_j^\mu|). \quad (3.56)$$

where $c \in \mathbb{C}$ and $s \in \mathbb{R}$. Since $a_i \neq a_j$, at least one side of a_i or a_j is different from x_k . Without loss of generality we assume $x_k \neq a_j$. Because of the Lemma 3, $\mathcal{I}_k(|a_j^\mu\rangle\langle a_j^\mu|) = 0$. Then

$$\mathcal{I}_k(\rho_+) = s^2 \mathcal{I}_k(|a_i^\lambda\rangle\langle a_i^\lambda|) + s \mathcal{I}_k(c|a_j^\mu\rangle\langle a_i^\lambda| + c^*|a_i^\lambda\rangle\langle a_j^\mu|), \quad (3.57)$$

$$\mathcal{I}_k(\rho_-) = s^2 \mathcal{I}_k(|a_i^\lambda\rangle\langle a_i^\lambda|) - s \mathcal{I}_k(c|a_j^\mu\rangle\langle a_i^\lambda| + c^*|a_i^\lambda\rangle\langle a_j^\mu|). \quad (3.58)$$

Since each \mathcal{I}_k is a CP map, both matrices $\mathcal{I}_k(\rho_+)$ and $\mathcal{I}_k(\rho_-)$ are positive matrices. Then for $s > 0$, it is easy to prove that

$$s \mathcal{I}_k(|a_i^\lambda\rangle\langle a_i^\lambda|) \geq \mathcal{I}_k(c|a_j^\mu\rangle\langle a_i^\lambda| + c^*|a_i^\lambda\rangle\langle a_j^\mu|) \geq -s \mathcal{I}_k(|a_i^\lambda\rangle\langle a_i^\lambda|). \quad (3.59)$$

By considering the limit $s \rightarrow 0+$, the middle side of Eq. (3.59) must be a zero matrix because of the pinching theorem. Therefore we obtain

$$\mathcal{I}_k(c|a_j^\mu\rangle\langle a_i^\lambda| + c^*|a_i^\lambda\rangle\langle a_j^\mu|) = 0. \quad (3.60)$$

Comparing the cases of $c = 1$ and $c = i$, we conclude Eq. (3.54). \square

Proof of Theorem. 2. Assume $R_1(\mathcal{M}|A) = 0$. Since Lemma 3, for all indices $i \in Y, j \in X$ satisfying $a_i \neq x_j$, $\mathcal{I}_j(|a_i^\lambda\rangle\langle a_i^\lambda|)$ becomes the zero matrix. Then

$$\sum_{j \in X} \mathcal{I}_j(|a_i^\lambda\rangle\langle a_i^\lambda|) = \sum_{j \in X_i} \mathcal{I}_j(|a_i^\lambda\rangle\langle a_i^\lambda|) = \tilde{\mathcal{I}}_{X_i}(|a_i^\lambda\rangle\langle a_i^\lambda|). \quad (3.61)$$

The projection superoperator \mathcal{P}_i^A satisfies

$$\mathcal{P}_i^A(|a_i^\lambda\rangle\langle a_i^\lambda|) = \delta_{i,j} |a_i^\lambda\rangle\langle a_i^\lambda| \quad (3.62)$$

by definition. Then by using Eqs.(3.61) and (3.62) $R_2(\mathcal{M}|A)$ for the extended measurement is calculated as

$$\begin{aligned} & R_2(\mathcal{M} \otimes \text{id}_{\mathcal{H}}|A \otimes I) \\ &= \sum_{i \in Y \cup \{0\}} \max_{\substack{\{ |a_i^\lambda\rangle \}, \{ |\psi_i^\lambda\rangle \} \\ \sum_{\lambda \in Z_i} |c_i^\lambda|^2 = 1}} \left\| \sum_{\lambda, \mu \in Z_i} c_i^{\lambda*} c_i^\mu \left(\tilde{\mathcal{I}}_{X_i}(|a_i^\lambda\rangle\langle a_i^\mu|) - \mathcal{P}_i^A(|a_i^\lambda\rangle\langle a_i^\mu|) \right) \otimes |\psi_i^\lambda\rangle\langle \psi_i^\mu| \right\|_{\text{tr}}, \end{aligned} \quad (3.63)$$

where $\{ |\psi_i^\lambda\rangle \}$ is a set of unit vectors on \mathcal{H} .

According to [34], a diamond norm of a CP map is calculated by maximization over all rank 1 density matrices instead of all the density matrices on $\mathcal{H} \otimes \mathcal{H}$. Thus

$$\left\| \tilde{\mathcal{I}}_{X_i} - \mathcal{P}_i^A \right\|_{\diamond} = \max_{\substack{|\Psi\rangle \in \mathcal{H} \otimes \mathcal{H} \\ \|\Psi\rangle\| = 1}} \left\| (\tilde{\mathcal{I}}_{X_i} - \mathcal{P}_i^A) \otimes \text{id}_{\mathcal{H}}(|\Psi\rangle\langle\Psi|) \right\|_{\text{tr}}. \quad (3.64)$$

A vector $|\Psi\rangle$ in $\mathcal{H} \otimes \mathcal{H}$ can be decomposed into a linear combination of vectors which is a tensor product of two unit vectors in \mathcal{H} by

$$|\Psi\rangle = \cos \theta \sum_{\lambda \in Z_i} c_i^\lambda |a_i^\lambda\rangle |\psi_i^\lambda\rangle + \sin \theta \sum_{\substack{j \neq i \\ \mu \in Z_j}} c_j^\mu |a_j^\mu\rangle |\psi_j^\mu\rangle. \quad (3.65)$$

By using Lemma 3, 4 and the property of the projection superoperator, we obtain

$$\begin{aligned} & \max_{|\Psi\rangle \in \mathcal{H} \otimes \mathcal{H}} \left\| (\tilde{\mathcal{I}}_{X_i} - \mathcal{P}_i^A) \otimes \text{id}_{\mathcal{H}} (|\Psi\rangle\langle\Psi|) \right\| \\ &= \max_{\theta \in [0, 2\pi]} \cos^2 \theta \max_{\substack{\{|a_i^\lambda\rangle\}, \{|\psi_i^\lambda\rangle\} \\ \sum_{\lambda \in Z_i} |c_i^\lambda|^2 = 1}} \left\| \sum_{\lambda, \mu \in Z_i} c_i^{\lambda*} c_i^\mu (\tilde{\mathcal{I}}_{X_i} - \mathcal{P}_i^A) (|a_i^\lambda\rangle\langle a_i^\mu|) \otimes |\psi_i^\lambda\rangle\langle\psi_i^\mu| \right\|_{\text{tr}} \\ &= \max_{\substack{\{|a_i^\lambda\rangle\}, \{|\psi_i^\lambda\rangle\} \\ \sum_{\lambda \in Z_i} |c_i^\lambda|^2 = 1}} \left\| \sum_{\lambda, \mu \in Z_i} c_i^{\lambda*} c_i^\mu (\tilde{\mathcal{I}}_{X_i} - \mathcal{P}_i^A) (|a_i^\lambda\rangle\langle a_i^\mu|) \otimes |\psi_i^\lambda\rangle\langle\psi_i^\mu| \right\|_{\text{tr}}. \quad (3.66) \end{aligned}$$

Then $R_2(\mathcal{M}, A)$ can be rewritten as

$$R_2(\mathcal{M} \otimes \text{id}_{\mathcal{H}} |A \otimes I) = \sum_{i \in Y} \left\| \tilde{\mathcal{I}}_{X_i} - \mathcal{P}_i^A \right\|_{\diamond}. \quad (3.67)$$

For any matrix $|a_k^\lambda\rangle\langle a_l^\mu|$, if $i \in X_0$, $\mathcal{I}_i(|a_k^\lambda\rangle\langle a_l^\mu|) = 0$ is satisfied due to Lemma 3 and Lemma 4. Because any matrix on $\mathcal{H} \otimes \mathcal{H}$ can be represented by a linear combination of these matrices, then

$$\tilde{\mathcal{I}}_{X_0} = \sum_{i \in A_0} \mathcal{I}_i = 0. \quad (3.68)$$

Since \mathcal{P}_0 is also the zero superoperator, we conclude the main result

$$R_2(\mathcal{M} \otimes \text{id} |A \otimes I) = \sum_{i \in Y \cup \{0\}} \left\| \tilde{\mathcal{I}}_{X_i} - \mathcal{P}_i^A \right\|_{\diamond} = D_{\diamond}(\tilde{\mathcal{I}}, \tilde{\mathcal{P}}). \quad (3.69)$$

On the other hand, when the observable A has no degeneracy degenerated, Eq. (3.66) becomes

$$\begin{aligned} \left\| \tilde{\mathcal{I}}_{X_i} - \mathcal{P}_i^A \right\|_{\diamond} &= \max_{|\Psi\rangle \in \mathcal{H} \otimes \mathcal{H}} \left\| (\tilde{\mathcal{I}}_{X_i} - \mathcal{P}_i^A) \otimes \text{id}_{\mathcal{H}} (|\Psi\rangle\langle\Psi|) \right\| \\ &= \left\| (\tilde{\mathcal{I}}_{X_i} - \mathcal{P}_i^A) (|a_i\rangle\langle a_i|) \otimes |\psi_i\rangle\langle\psi_i| \right\|_{\text{tr}} \\ &= \left\| (\tilde{\mathcal{I}}_{X_i} - \mathcal{P}_i^A) (|a_i\rangle\langle a_i|) \right\|_{\text{tr}}. \quad (3.70) \end{aligned}$$

Taking the summation of the above equality over $i \in Y$, we obtain the following equality of the degenerated case.

$$R_2(\mathcal{M} |A) = D_{\diamond}(\tilde{\mathcal{I}}, \tilde{\mathcal{P}}) = D_{\diamond}(\mathcal{M}, \mathcal{M}^A). \quad (3.71)$$

□

Next, we prove Theorem 3. We prepare the following five lemmas for proving the theorem.

Lemma 5. For a measurement $\mathcal{M} = \{\mathcal{I}, x, X\}$, let us define $e_{i,\lambda,k}$ by

$$\mathrm{Tr} \left[\mathcal{I}_k(|a_i^\lambda\rangle\langle a_i^\lambda|) \right] = \frac{e_{i,\lambda,k}}{(x_k - a_i)^2}. \quad (3.72)$$

This $e_{i,\lambda,k}$ satisfies

$$\sum_{k \in X} e_{i,\lambda,k} < R_1(\mathcal{M}|A), \quad e_{i,\lambda,k} > 0. \quad (3.73)$$

Proof. The proof of this lemma is almost trivial. Because of the definition of $R_1(\mathcal{M}|A)$

$$\begin{aligned} \sum_{k \in X} e_{i,\lambda,k} &= \sum_{k \in X} \mathrm{Tr} \left[\mathcal{I}_k(|a_i^\lambda\rangle\langle a_i^\lambda|) \right] (a_i - x_k)^2 \\ &\leq \max_{\substack{\{|a_i^\lambda\rangle\} \\ i \in Y, \lambda \in Z_i}} \sum_{k \in X} \mathrm{Tr} \left[\mathcal{I}_k(|a_i^\lambda\rangle\langle a_i^\lambda|) \right] (a_i - x_k)^2 \\ &= R_1(\mathcal{M}|A). \end{aligned} \quad (3.74)$$

□

To prove the rest of lemmas, we define a subspace $\mathcal{H}_{i,\lambda} = \mathrm{span}\{|a_i^\lambda\rangle\}$ for any eigen state $|a_i^\lambda\rangle$ of an observable A . We also denote the effect of a CP map \mathcal{I}_k as

$$\mathcal{I}_k(|a_i^\lambda\rangle\langle a_i^\lambda|) = q_{i,\lambda,k}|a_i^\lambda\rangle\langle a_i^\lambda| + r_{i,\lambda,k}\sigma_{i,\lambda,k} + \xi_{i,\lambda,k}. \quad (3.75)$$

where $\sigma_{i,\lambda,k}$ is a density matrix on $\mathcal{H}_{i,\lambda}^\perp$, $q_{i,\lambda,k}, r_{i,\lambda,k}$ are positive real numbers and $\xi_{i,\lambda,k}$ is a traceless Hermite operator which can be decomposed as

$$|\psi_{i,\lambda,k}\rangle \in \mathcal{H}_{i,\lambda}^\perp, \quad \xi_{i,\lambda,k} = (|a_i^\lambda\rangle\langle\psi_{i,\lambda,k}| + |\psi_{i,\lambda,k}\rangle\langle a_i^\lambda|). \quad (3.76)$$

Lemma 6. For a measurement $\mathcal{M} = \{\mathcal{I}, x, X\}$,

$$2 \sum_k r_{i,\lambda,k} \leq R_2(\mathcal{M}|A) \quad (3.77)$$

is satisfied for all $i \in Y, \lambda \in Z_i$ and $k \in X$.

Proof. To prove this lemma, note that the trace norm satisfies monotonicity condition [34] as $\|\rho - \sigma\|_{\mathrm{tr}} > \|\Lambda\rho - \Lambda\sigma\|_{\mathrm{tr}}$ for any CPTP map Λ , where ρ and σ are two density matrices. We define projectors $P_{i,\lambda}$ and $P_{i,\lambda}^\perp$ which is onto the subspaces $\mathcal{H}_{i,\lambda}$ and $\mathcal{H}_{i,\lambda}^\perp$. We define the following CPTP map $\Lambda_{i,\lambda}$ as

$$\Lambda_{i,\lambda}(\rho) = P_{i,\lambda}\rho P_{i,\lambda} + P_{i,\lambda}^\perp\rho P_{i,\lambda}^\perp. \quad (3.78)$$

The monotonicity of the trace norm leads to

$$\left\| \Lambda_{i,\lambda} \left(\Lambda_{\mathcal{I}}(|a_i^\lambda\rangle\langle a_i^\lambda|) - |a_i^\lambda\rangle\langle a_i^\lambda| \right) \right\|_{\text{tr}} \leq \left\| \Lambda_{\mathcal{I}}(|a_i^\lambda\rangle\langle a_i^\lambda|) - |a_i^\lambda\rangle\langle a_i^\lambda| \right\|_{\text{tr}}. \quad (3.79)$$

According to the definition of $R_2(\mathcal{M}|A)$, the left-hand side of the above equation is bounded by $R_2(\mathcal{M}|A)$ as

$$\left\| \Lambda_{i,\lambda} \left(\Lambda_{\mathcal{I}}(|a_i^\lambda\rangle\langle a_i^\lambda|) - |a_i^\lambda\rangle\langle a_i^\lambda| \right) \right\|_{\text{tr}} \leq R_2(\mathcal{M}|A). \quad (3.80)$$

Substituting the definition of $\Lambda_{\mathcal{I}}$ in this inequality, we obtain

$$\left\| \Lambda_{i,\lambda} \left(\sum_k \mathcal{I}_k(|a_i^\lambda\rangle\langle a_i^\lambda|) - |a_i^\lambda\rangle\langle a_i^\lambda| \right) \right\|_{\text{tr}} = \left\| \sum_{k \in X} \left(r_{i,\lambda,k} \sigma_{i,\lambda,k} - (1 - q_{i,\lambda,k}) |a_i^\lambda\rangle\langle a_i^\lambda| \right) \right\|_{\text{tr}}. \quad (3.81)$$

Because of the definition of a density matrix and a CPTP map, we can derive a relationship between coefficients $q_{i,\lambda,k}$ and $r_{i,\lambda,k}$ by

$$\text{Tr} [\Lambda_{\mathcal{I}} \rho] = \sum_{k \in X} (q_{i,\lambda,k} + r_{i,\lambda,k}) = 1. \quad (3.82)$$

Then the sum of $1 - q_{i,\lambda,k}$ satisfies

$$\sum_{k \in X} (1 - q_{i,\lambda,k}) = \sum_{k \in X} r_{i,\lambda,k}. \quad (3.83)$$

Substituting this value in Eq. (3.81), we obtain

$$\left\| \Lambda_{i,\lambda} \left(\Lambda_{\mathcal{I}}(|a_i^\lambda\rangle\langle a_i^\lambda|) - |a_i^\lambda\rangle\langle a_i^\lambda| \right) \right\|_{\text{tr}} = \left\| \sum_{k \in X} r_{i,\lambda,k} \left(\sigma_{i,\lambda,k} - |a_i^\lambda\rangle\langle a_i^\lambda| \right) \right\|_{\text{tr}}. \quad (3.84)$$

Because the trace norm of an Hermitian operator is calculated as the sum of the absolute value of its eigenvalues [36], if a matrix is given as the sum of the two different matrices on orthogonal subspaces, its trace norm becomes the sum of each trace norm, namely,

$$\left\| \sum_{k \in X} r_{i,\lambda,k} \left(\sigma_{i,\lambda,k} - |a_i^\lambda\rangle\langle a_i^\lambda| \right) \right\|_{\text{tr}} = \left\| \sum_{k \in X} r_{i,\lambda,k} \sigma_{i,\lambda,k} \right\|_{\text{tr}} + \left\| \sum_{k \in X} r_{i,\lambda,k} |a_i^\lambda\rangle\langle a_i^\lambda| \right\|_{\text{tr}}. \quad (3.85)$$

Due to the same reason, the trace norm of a linear combination of positive matrices has linearity, then

$$\begin{aligned} \left\| \sum_{k \in X} r_{i,\lambda,k} \sigma_{i,\lambda,k} \right\|_{\text{tr}} + \left\| \sum_{k \in X} r_{i,\lambda,k} |a_i^\lambda\rangle\langle a_i^\lambda| \right\|_{\text{tr}} \\ = \sum_{k \in X} r_{i,\lambda,k} \left\| \sigma_{i,\lambda,k} \right\|_{\text{tr}} + \sum_{k \in X} r_{i,\lambda,k} \left\| |a_i^\lambda\rangle\langle a_i^\lambda| \right\|_{\text{tr}}. \end{aligned} \quad (3.86)$$

Since the trace norm of a density matrix is equal to 1, the left-hand side of the above equation is $2 \sum_{k \in X} r_{i,\lambda;k}$. Then we can simplify the left-hand side of Eq. (3.80) as

$$2 \sum_{k \in X} r_{i,\lambda;k} \leq R_2(\mathcal{M}|A). \quad (3.87)$$

□

Lemma 7. For any completely positive map \mathcal{I} on a Hilbert space \mathcal{H} ,

$$|\langle \chi | \mathcal{I}(|\psi\rangle\langle\phi|) | \chi \rangle| \leq \sqrt{\langle \chi | \mathcal{I}(|\psi\rangle\langle\psi|) | \chi \rangle \langle \chi | \mathcal{I}(|\phi\rangle\langle\phi|) | \chi \rangle} \quad (3.88)$$

is satisfied for any $|\psi\rangle, |\phi\rangle, |\chi\rangle \in \mathcal{H}$.

Proof. A binary operation $(|\psi\rangle, |\phi\rangle) = \langle \chi | (\mathcal{I}|\psi\rangle\langle\phi|) | \chi \rangle$ satisfies the some property of the inner product except the non-degeneracy condition

$$(|\psi\rangle, |\psi\rangle) = 0 \Rightarrow |\psi\rangle = 0. \quad (3.89)$$

The Cauchy-Schwartz inequality of inner product is still valid for binary operation without this condition. Then this Lemma is satisfied. □

Lemma 8. For a measurement $\mathcal{M} = \{\mathcal{I}, x, X\}$ and a real function f satisfying $0 \leq |f| \leq \Delta$, the following is satisfied for any $k \in X$, $i, j \in Y$ satisfying $i \neq j$,

$$\left| \text{Tr} \left[\mathcal{I}(f)(|a_i^\lambda\rangle\langle a_j^\mu|) \right] \right| \leq \Delta \left(\sqrt{2R_2(\mathcal{M}|A)} + \frac{R_2(\mathcal{M}|A)}{2} \right). \quad (3.90)$$

Proof. Because of the triangular inequality of the absolute value, the left-hand side of Eq. (3.90) is bounded as

$$\begin{aligned} \left| \text{Tr} \left[\mathcal{I}(f)(|a_i^\lambda\rangle\langle a_j^\mu|) \right] \right| &= \left| \sum_{l \in Y, \alpha \in Z} \langle a_l^\alpha | \mathcal{I}(f)(|a_j^\mu\rangle\langle a_i^\lambda|) | a_l^\alpha \rangle \right| \\ &\leq \sum_{l \in Y, \alpha \in Z} \left| \langle a_l^\alpha | \mathcal{I}(f)(|a_j^\mu\rangle\langle a_i^\lambda|) | a_l^\alpha \rangle \right| \end{aligned}$$

By using Lemma 7, we have

$$\begin{aligned} &\sum_{l \in Y, \alpha \in Z} \left| \langle a_l^\alpha | \mathcal{I}(f)(|a_j^\mu\rangle\langle a_i^\lambda|) | a_l^\alpha \rangle \right| \\ &\leq \sum_{l \in Y, \alpha \in Z} \sqrt{\langle a_l^\alpha | \mathcal{I}(f)(|a_i^\lambda\rangle\langle a_i^\lambda|) | a_l^\alpha \rangle} \times \sqrt{\langle a_l^\alpha | \mathcal{I}(f)(|a_j^\mu\rangle\langle a_j^\mu|) | a_l^\alpha \rangle}. \quad (3.91) \end{aligned}$$

We devide the summation of the right-hand side of Eq. (3.91) into two cases, one is that the combinations of indices satisfy $(l, \alpha) \neq (i, \lambda), (j, \mu)$ and the other

consists of the rest combinations. Using Eq. (3.75), the sum of the former combinations is represented as

$$\begin{aligned} & \sum_{\substack{(l,\alpha) \neq \\ (i,\lambda),(j,\mu)}} \sqrt{\langle a_l^\alpha | \mathcal{I}(f) | a_i^\lambda \rangle \langle a_i^\lambda | a_l^\alpha \rangle} \sqrt{\langle a_l^\alpha | \mathcal{I}(f) | a_j^\mu \rangle \langle a_j^\mu | a_l^\alpha \rangle} \\ &= \sum_{\substack{(l,\alpha) \neq \\ (i,\lambda),(j,\mu)}} \sqrt{\sum_k f(x_k) r_{i,\lambda;k} \langle a_l^\alpha | \sigma_{i;k} | a_l^\alpha \rangle} \sqrt{\sum_h f(x_h) r_{j,\mu;h} \langle a_l^\alpha | \sigma_{j;h} | a_l^\alpha \rangle}. \end{aligned}$$

Applying Cauchy-Schwartz's inequality to the right-hand side of the above equality, then we obtain

$$\begin{aligned} & \sum_{\substack{(l,\alpha) \neq \\ (i,\lambda),(j,\mu)}} \sqrt{\sum_k f(x_k) r_{i,\lambda;k} \langle a_l^\alpha | \sigma_{i;k} | a_l^\alpha \rangle} \sqrt{\sum_h f(x_h) r_{j,\mu;h} \langle a_l^\alpha | \sigma_{j;h} | a_l^\alpha \rangle} \\ & \leq \sqrt{\sum_k f(x_k) r_{i,\lambda;k} \sum_{\substack{(l,\alpha) \neq \\ (i,\lambda),(j,\mu)}} \langle a_l^\alpha | \sigma_{i;k} | a_l^\alpha \rangle} \sqrt{\sum_h f(x_h) r_{j,\mu;h} \sum_{\substack{(m,\beta) \neq \\ (i,\lambda),(j,\mu)}} \langle a_m^\beta | \sigma_{j;h} | a_m^\beta \rangle}. \end{aligned}$$

Substituting the following conditions

$$0 \leq f \leq \Delta, \quad 0 \leq \sum_{\substack{(l,\alpha) \neq \\ (i,\lambda),(j,\mu)}} \langle a_l^\alpha | \sigma_{i;k} | a_l^\alpha \rangle \leq 1, \quad (3.92)$$

the equation is bounded as

$$\begin{aligned} & \sqrt{\sum_k f(x_k) r_{i,\lambda;k} \sum_{\substack{(l,\alpha) \neq \\ (i,\lambda),(j,\mu)}} \langle a_l^\alpha | \sigma_{i;k} | a_l^\alpha \rangle} \sqrt{\sum_h f(x_h) r_{j,\mu;h} \sum_{\substack{(m,\beta) \neq \\ (i,\lambda),(j,\mu)}} \langle a_m^\beta | \sigma_{j;h} | a_m^\beta \rangle} \\ & \leq \Delta \sqrt{\sum_k r_{i,\lambda;k}} \sqrt{\sum_h r_{j,\mu;h}} \leq \frac{R_2(\mathcal{M}|A)}{2} \Delta. \end{aligned}$$

The last line is derived from Lemma 6. By using the same conditions, the rest part of the summation in the left-hand side of Eq. (3.91) is bounded as

$$\begin{aligned} & \sum_{\substack{(l,\alpha) = \\ (i,\lambda) \text{ or } (j,\mu)}} \sqrt{\sum_k f(x_k) r_{i,\lambda;k} \langle a_l^\alpha | \sigma_{i;k} | a_l^\alpha \rangle} \sqrt{\sum_h f(x_h) r_{j,\mu;h} \langle a_l^\alpha | \sigma_{j;h} | a_l^\alpha \rangle} \\ & \leq \Delta \left(\sqrt{\sum_k r_{j,\mu;k}} + \sqrt{\sum_h r_{i,\lambda;h}} \right) \leq \Delta \sqrt{2R_2(\mathcal{M}|A)}. \end{aligned}$$

The last line is also derived from Lemma 6. Combining all the inequalities, we obtain

$$\left| \text{Tr} \left[\mathcal{I}(f) (|a_i^\lambda\rangle\langle a_j^\mu|) \right] \right| \leq \Delta \left(\sqrt{2R_2(\mathcal{M}|A)} + \frac{R_2(\mathcal{M}|A)}{2} \right). \quad (3.93)$$

□

Lemma 9. For an observable A , we define its eigenbasis as $\{|a_i^\lambda\rangle | i \in Y, \lambda \in Z\}$, where $|a_i^\lambda\rangle$ is an eigenstate corresponding to an eigenvalue a_i . Let us denote by P_i^λ as the projective operator onto the subspace $\mathcal{H}_i^\lambda = \text{span}\{|a_i^\lambda\rangle\}$. We define a projective superoperator $\mathcal{P}_i^\lambda \rho = P_i^\lambda \rho P_i^\lambda$. For a measurement $\mathcal{M} = \{\mathcal{I}, x, X\}$ and a real function f satisfying $0 \leq f \leq \Delta$,

$$\left| \text{Tr} \left[\mathcal{I}(f) \left(\text{id} - \sum_{l \in Y, \alpha \in Z} \mathcal{P}_l^\alpha \right) (|\psi\rangle\langle\psi|) \right] \right| \leq d\Delta \left(\sqrt{2R_2(\mathcal{M}|A)} + \frac{R_2(\mathcal{M}|A)}{2} \right), \quad (3.94)$$

is satisfied for any unitvector $|\psi\rangle \in \mathcal{H}$, where $d = \dim \mathcal{H}$.

Proof. We decompose a unit vector $|\psi\rangle \in \mathcal{H}$ in the eigenbasis $\{|a_i^\lambda\rangle\}$ of A as

$$|\psi\rangle = \sum_{i,\lambda} e^{i\theta_i^\lambda} c_i^\lambda |a_i^\lambda\rangle, \quad c_i \in \mathbb{R}, \quad c_i > 0, \quad (3.95)$$

$$\sum_{i,\lambda} (c_i^\lambda)^2 = 1. \quad (3.96)$$

By using this notation, we can decompose $|\psi\rangle\langle\psi|$ as

$$\left(\text{id} - \sum_{l \in Y, \alpha \in Z} \mathcal{P}_l^\alpha \right) (|\psi\rangle\langle\psi|) = \sum_{\substack{(i,\lambda) \\ \neq (j,\mu)}} c_i^\lambda c_j^\mu e^{i(\theta_i^\lambda - \theta_j^\mu)} |a_i^\lambda\rangle\langle a_j^\mu|. \quad (3.97)$$

Then

$$\begin{aligned} \left| \text{Tr} \left[\mathcal{I}_k \left(\text{id} - \sum_{l \in Y, \alpha \in Z} \mathcal{P}_l^\alpha \right) (|\psi\rangle\langle\psi|) \right] \right| &\leq \sum_{(i,\lambda) \neq (j,\mu)} c_i^\lambda c_j^\mu \left| \mathcal{I}(f) (|a_i^\lambda\rangle\langle a_j^\mu|) \right| \\ &\leq \Delta \sum_{(i,\lambda) \neq (j,\mu)} c_i^\lambda c_j^\mu \left(\sqrt{2R_2(\mathcal{M}|A)} + \frac{R_2(\mathcal{M}|A)}{2} \right) \\ &\leq \Delta \sum_{i,\lambda} c_i^\lambda \sum_{j,\mu} c_j^\mu \left(\sqrt{2R_2(\mathcal{M}|A)} + \frac{R_2(\mathcal{M}|A)}{2} \right) \\ &\leq d\Delta \left(\sqrt{2R_2(\mathcal{M}|A)} + \frac{R_2(\mathcal{M}|A)}{2} \right). \end{aligned} \quad (3.98)$$

From the second line to the third line, we used Lemma 8. From the second last line to the last line, we used the fact that the maximum value of $\sum_{i,\lambda} c_i^\lambda$ under the condition Eq. (3.96) is given when all coefficients c_i^λ are $1/\sqrt{d}$. (This fact is easily proven by using the concavity of the square function.) □

Lemma 10. For a measurement $\mathcal{M} = \{I, x, X\}$ and an observable A ,

$$\left| \text{Tr} \left[(I(f) - \mathcal{P}(f)) \sum_{l \in Y, \alpha \in Z} \mathcal{P}_l^\alpha (|\psi\rangle\langle\psi|) \right] \right| < 2 \sqrt{R_1(\mathcal{M}|A)}, \quad (3.99)$$

for any state $|\psi\rangle \in \mathcal{H}$, where f is chosen as a Lipschitz function.

Proof. We first evaluate the following value.

$$\begin{aligned} \left| \text{Tr} \left[(I(f) - \mathcal{P}(f)) (|a_i^\lambda\rangle\langle a_i^\lambda|) \right] \right| &= \left| \sum_{l \in Y, \alpha \in Z} \langle a_l^\alpha | (I(f) - \mathcal{P}(f)) (|a_i^\lambda\rangle\langle a_i^\lambda|) |a_l^\alpha\rangle \right| \\ &= \left| \sum_k (f(x_k) - f(a_i)) \sum_{l \in Y, \alpha \in Z} \langle a_l^\alpha | \mathcal{I}_k (|a_i^\lambda\rangle\langle a_i^\lambda|) |a_l^\alpha\rangle \right| \\ &\leq \sum_k |f(x_k) - f(a_i)| \sum_{l \in Y, \alpha \in Z} \langle a_l^\alpha | \mathcal{I}_k (|a_i^\lambda\rangle\langle a_i^\lambda|) |a_l^\alpha\rangle \end{aligned} \quad (3.100)$$

We define the following set of the measurement values of \mathcal{M} ,

$$C_i = \{k \in X | |a_i - x_k| \leq \sqrt{R_1(\mathcal{M}|A)}\} \quad (3.101)$$

We split the summation of Eq. (3.100) into the indices included in C_i and the others. The former part is evaluated as

$$\begin{aligned} \sum_{k \in C_i} |f(x_k) - f(a_i)| \sum_{l \in Y, \alpha \in Z} \langle a_l^\alpha | (\mathcal{I}_k(f) - \mathcal{P}_i) (|a_i^\lambda\rangle\langle a_i^\lambda|) |a_k^\alpha\rangle \\ \leq \sqrt{R_1(\mathcal{M}|A)} \sum_{l \in C_i} \langle a_l^\alpha | \sum_k \mathcal{I}_k (|a_i^\lambda\rangle\langle a_i^\lambda|) |a_l^\alpha\rangle \\ \leq \sqrt{R_1(\mathcal{M}|A)} \text{Tr} \left[\sum_k \mathcal{I}_k (|a_i^\lambda\rangle\langle a_i^\lambda|) \right] = \sqrt{R_1(\mathcal{M}|A)}. \end{aligned} \quad (3.102)$$

The other part is calculated as

$$\sum_{k \notin C_i} |f(x_k) - f(a_i)| \left| \sum_{l \in Y, \alpha \in Z} \langle a_l^\alpha | (\mathcal{I}_k - \mathcal{P}_i) (|a_i^\lambda\rangle\langle a_i^\lambda|) |a_k^\alpha\rangle \right| \leq \sum_{k \in C_i} e_{i,k} \frac{|f(x_k) - f(a_i)|}{(x_k - a_i)^2} \quad (3.103)$$

Note that for any $k \notin C_i$,

$$R_1(\mathcal{M}|A) |x_k - a_i| \leq (x_k - a_i)^2 \quad (3.104)$$

is satisfied. Then

$$\sum_{k \in C_i} e_{i,k} \frac{|f(x_k) - f(a_i)|}{(x_k - a_i)^2} \leq \frac{1}{\sqrt{R_1(\mathcal{M}|A)}} \sum_{k \in C_i} e_{i,k} \leq \sqrt{R_1(\mathcal{M}|A)}. \quad (3.105)$$

We used the definition of the Lipschitz function and Lemma 5 to derive the second line from the first line. Then, the summations of indices of $k \in C_i$ and of $k \notin C_i$ are given. The total is given by

$$\left| \text{Tr} \left[(\mathcal{I}(f) - \mathcal{P}(f)) |a_i^\lambda\rangle\langle a_i^\lambda| \right] \right| < 2 \sqrt{R_1(\mathcal{M}|A)}. \quad (3.106)$$

For any unit vector $|\psi\rangle \in \mathcal{H}$ defined in Eq. (3.95) and (3.96),

$$\sum_{l \in Y, \alpha \in Z} \mathcal{P}_l^\alpha |\psi\rangle\langle\psi| = \sum_{l \in Y, \alpha \in Z} (c_l^\alpha)^2 |a_l^\alpha\rangle\langle a_l^\alpha| \quad (3.107)$$

is satisfied. Then

$$\begin{aligned} \left| [(\mathcal{I}(f) - \mathcal{P}(f)) \sum_{l \in Y, \alpha \in Z} \mathcal{P}_l^\alpha |\psi\rangle\langle\psi|] \right| &\leq \sum_{i, \lambda} (c_i^\lambda)^2 \left| \text{Tr} [(\mathcal{I}(f) - \mathcal{P}(f)) |a_i^\lambda\rangle\langle a_i^\lambda|] \right| \\ &\leq 2 \sqrt{R_1(\mathcal{M}|A)} \sum_{i, \lambda} (c_i^\lambda)^2 \\ &= 2 \sqrt{R_1(\mathcal{M}|A)}. \end{aligned} \quad (3.108)$$

Therefore the Lemma 10 is proven. \square

Proof of Theorem 3. By definition, the Monge distance between \mathcal{M} and \mathcal{M}^A is defined as

$$\|\mathcal{M} - \mathcal{M}^A\|_m := \sup_{\substack{\rho \in D(\mathcal{H}) \\ f \in L}} \left| \text{Tr} [(\mathcal{I}(f) - \mathcal{P}(f)) \rho] \right| \quad (3.109)$$

The functional which has been maximized in the right-hand side of the above equation is translationally invariant. For a Lipschitz function f , we define its parallel translation f' by a constant $c \in \mathbb{R}$ as

$$f'(x) = f(x) + c. \quad (3.110)$$

Then f and f' satisfy

$$\left| \text{Tr} [(\mathcal{I}(f') - \mathcal{P}(f')) \rho] \right| = \left| \text{Tr} [(\mathcal{I}(f) - \mathcal{P}(f)) \rho] \right| \quad (3.111)$$

This relationship is derived from the condition required for measurement instruments, namely,

$$\text{Tr} [\mathcal{I}(1) \rho] = \text{Tr} [\mathcal{P}(1) \rho] = 1. \quad (3.112)$$

Therefore without losing generality, we can assume the condition for a Lipschitz function f given by

$$\forall i \in X, \quad \Delta x_{\max} \geq f(x_i) \geq 0. \quad (3.113)$$

We denote the diagonalization of a density matrix ρ as

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|, \quad \sum_i p_i = 1, \quad p_i \geq 0. \quad (3.114)$$

Using the triangular inequality, we achieve the upper bound of a term in the right-hand side of Eq. (3.109) as follows.

$$|\text{Tr}[(\mathcal{I}(f) - \mathcal{P}(f))\rho]| \leq \sum_i p_i |\text{Tr}[(\mathcal{I}(f) - \mathcal{P}(f))(|\psi_i\rangle\langle\psi_i|)]|. \quad (3.115)$$

Because of its definition $\mathcal{P}(f)$ satisfies

$$\text{Tr}[\mathcal{P}(f)\mathcal{P}_i^\alpha\rho] = \text{Tr}[\mathcal{P}(f)\rho], \quad (3.116)$$

for any density matrix ρ on \mathcal{H} . Then we achieve

$$\text{Tr}[(\mathcal{I}(f) - \mathcal{P}(f))\rho] = \text{Tr}[(\mathcal{I}(f) - \mathcal{P}(f))\mathcal{P}_i^\alpha\rho] - \text{Tr}[\mathcal{I}(f)(id - \mathcal{P}_i^\alpha(f))\rho] \quad (3.117)$$

Substituting this equation into a term in the right-hand side of Eq. (3.115) and applying the triangular inequality, we derive

$$\begin{aligned} & \left| [(\mathcal{I}(f) - \mathcal{P}(f))(|\psi_i\rangle\langle\psi_i|)] \right| \\ & \leq \left| \text{Tr} \left[(\mathcal{I}(f) - \mathcal{P}(f)) \sum_{l \in Y, \alpha \in Z} \mathcal{P}_l^\alpha(|\psi_i\rangle\langle\psi_i|) \right] \right| + \left| \text{Tr} \left[\mathcal{I}(f) \left(id - \sum_{l \in Y, \alpha \in Z} \mathcal{P}_l^\alpha \right) (|\psi_i\rangle\langle\psi_i|) \right] \right|. \end{aligned} \quad (3.118)$$

Applying Lemmas 9 and 10 for the right-hand side of the above inequality, we have

$$\left| [(\mathcal{I}(f) - \mathcal{P}(f))(|\psi_i\rangle\langle\psi_i|)] \right| \leq 2\sqrt{R_1(\mathcal{M}|A)} + d\Delta x_{max} \left(\sqrt{2R_2(\mathcal{M}, A)} + \frac{R_2(\mathcal{M}, A)}{2} \right), \quad (3.119)$$

where we use the condition Eq. (3.113) to apply Lemma 9. Then we can reformulate Eq. (3.115) as

$$\left| [(\mathcal{I}(f) - \mathcal{P}(f))\rho] \right| \leq 2\sqrt{R_1(\mathcal{M}|A)} + d\Delta x_{max} \left(\sqrt{2R_2(\mathcal{M}, A)} + \frac{R_2(\mathcal{M}, A)}{2} \right). \quad (3.120)$$

Because of Eq. (3.109), we achieve the upper bound of the Monge distance as

$$\|\mathcal{M} - \mathcal{M}^A\|_m \leq 2\sqrt{R_1(\mathcal{M}|A)} + d\Delta x_{max} \left(\sqrt{2R_2(\mathcal{M}, A)} + \frac{R_2(\mathcal{M}, A)}{2} \right). \quad (3.121)$$

thus we have proven the Theorem. 3. \square

Chapter 4

Tomography-based method: approach and evaluation

4.1 Introduction

For a quantum system evolving according to the Schrödinger equation determined by an unknown Hamiltonian, a straightforward way to implement the projective measurement of energy is given as follows. First, we somehow identify the Hamiltonian by estimation. Next, we perform the projective measurement of energy of the estimated Hamiltonian. To identify a Hamiltonian, we must first identify the Hamiltonian dynamics, and we estimate the generator of the dynamics afterwards. The general method to identify quantum dynamics is called process tomography [35], which determines an unknown CPTP by preparing many copies of initial states and executing many runs of measurements on the states affected by the map. However the process tomography is not only valid for Hamiltonian dynamics but it is also applicable for all dynamics represented by CPTP maps, which is identified by $d^4 - d^2$ parameters. Because a unitary operator is determined by $(d^2 + 1)/2$ independent parameters, the general process tomography requires excess cost for just identifying Hamiltonian dynamics. However the tomography method which only focuses on the unitary dynamics has not been well established.

In this chapter, we propose a process tomography purely for determining a unitary dynamics and apply this method to implement the projective measurement of energy. In Sec. 4.2, we introduce the basics of estimation. In Sec. 4.3, we construct a process tomography to identify a unitary operator. In Sec. 4.4, we introduce a method to implement the energy eigenbasis measurement from the result of estimation.

4.2 Estimation theory

In natural science, we describe a state by a set of numbers called parameters. We call such numbers as parameters of the state. States described by different values of parameters respond differently in observations. The trial of an observation is a stochastic subject, and they are to be written by random variables. This relationship between a parameter and stochastic trials can be described as followings.

Definition 22. Consider a random variable $x \in \mathbb{R}$ whose probability distributions $p_\theta(x)$ is dependent on a vector of complex numbers θ , where

$$\theta = (\theta_1, \theta_2, \dots, \theta_N)^T, \quad \theta_i \in \mathbb{C}. \quad (4.1)$$

We call this θ as the parameter of the probability distribution.

We call a process reconstructing an unknown parameter from a set of data obtained by stochastic trials as an estimation. A function which transforms a set of data into a possible parameter is called an estimator.

Definition 23. Consider there are K random variables $\{x^{(k)} | 1 \leq k \leq K\}$, the probability distribution of $x^{(k)}$ is denoted as $p_\theta^{(k)}$ which depends on the parameter $\theta \in \mathbb{C}^N$. We iterate stochastic trials of each random variable $x^{(k)}$ M_k times. Let us denote the data of the m -th trial of the k -th random variable $x^{(k)}$ as $d_m^{(k)}$. We denote a set of data of all the trials as $D = \{D^{(1)}, D^{(2)}, \dots, D^{(K)}\}$, where $D^{(k)} = \{d_1^{(k)}, d_2^{(k)}, \dots, d_{M_k}^{(k)}\}$.

Definition 24. We define a function $\theta^{(est)} : S \rightarrow \mathbb{C}^N$, where the set S includes all possible set of data D of stochastic trials depending on the parameter θ . We refer to this function as an estimator.

As an example of an estimator, we introduce the linear estimator. To formulate this function, we first define the sample mean of a set of data.

Definition 25. For a set of data $D = \{D^{(1)}, D^{(2)} \dots\}$, we define the sample mean of the data of the random variable $x^{(k)}$ as

$$\langle D^{(k)} \rangle^{\text{ave}} = \frac{1}{M^{(k)}} \sum_i d_i^{(k)}. \quad (4.2)$$

For any function f , we denote the sample mean of $f(d_i^{(k)})$ as

$$\langle f \rangle_{D^{(k)}}^{\text{ave}} = \frac{1}{M^{(k)}} \sum_i f(d_i^{(k)}). \quad (4.3)$$

Definition 26. Let us define a set of data of the stochastic trials as D . The estimator in the following form is called linear estimator:

$$\theta_i^{\text{est}}(D) = \sum_{k,i} \langle f_i^{(k)} \rangle_{D^{(k)}}^{\text{ave}}, \quad (4.4)$$

where

$$f_i^{(k)} : \mathbb{R} \rightarrow \mathbb{C}. \quad (4.5)$$

The linear estimator is for estimating the parameter given by a linear combination of the expectation value of trials. The expectation value is given as follows.

Definition 27. For a random variable x of which probability distribution is given by $p_\theta(x)$, we define the expectation value of the random variable by

$$\langle x \rangle_\theta^{\text{exp}} = \sum_x p_\theta(x)x. \quad (4.6)$$

For any real function f , we also define the expectation value by

$$\langle f \rangle_{x,\theta}^{\text{exp}} := \sum_x p_\theta(x) f(x). \quad (4.7)$$

To evaluate how close each of estimated value $\theta^{(\text{est})}(D)$ to θ is, we generally adopt some two-variable functions, which are called loss functions.

Definition 28. We call a two variable function $\Delta : \mathbb{C} \times \mathbb{C} \rightarrow \mathbb{R}$ satisfying the following conditions for any $a, b, c \in \mathbb{R}^N$ a loss function for a parameter.

1. $\Delta(a, b) \geq 0$. (Positivity)
2. $\Delta(a, a) = 0$.
3. $\Delta(a, b) = \Delta(b, a)$. (Symmetry)
4. $\Delta(a, c) \leq \Delta(a, b) + \Delta(b, c)$. (Triangle inequality).

As a loss function, we define the squared error defined as follows.

Definition 29. A two variable function Δ_2 is defined by

$$\Delta_2(a, b) := |a - b|^2, \quad (4.8)$$

where $a, b \in \mathbb{C}$. This function is called the squared error. We also define a generalized version of this loss function by

$$\Delta_n(a, b) := |a - b|^n. \quad (4.9)$$

Since the data of trials are obtained probabilistically, thus the outcome of the estimator behaves also probabilistically. The estimator of which estimated value gives a small loss function in typical cases should be a good estimator. To evaluate probabilistic behavior of an estimator, we introduce the following two quantities. The first is the expected loss, which is the average value of the loss function. The second is the error probability which can be regarded as the probability that the loss function larger than ε is achieved.

Definition 30. Expected loss of the i -th element of an estimator $\theta^{(\text{est})}$ for a loss function Δ is defined as

$$\Delta_2^{\text{exp}}(\theta_i^{\text{est}}) = \left\langle \Delta_2(\theta_i^{\text{est}}(D), \theta_i) \right\rangle_{D,\theta}^{\text{exp}}, \quad (4.10)$$

where

$$\left\langle \Delta(\theta_i^{\text{est}}(D), \theta_i) \right\rangle_{D,\theta}^{\text{exp}} = \sum_{D \in \mathcal{S}} \prod_{k,j} p_\theta^{(k)}(d_j^{(k)}) \Delta(\theta_i^{\text{est}}(D), \theta_i). \quad (4.11)$$

Definition 31. Define a step function $s_i^{(\varepsilon, \theta)}$ for an estimator θ^{est} as

$$s_i^{(\varepsilon, \theta)}(D) = 0 \quad (\Delta(\theta_i^{\text{est}}(D), \theta_i) < \varepsilon) \quad (4.12)$$

$$= 1 \quad (\Delta(\theta_i^{\text{est}}(D), \theta_i) \geq \varepsilon). \quad (4.13)$$

For an error ε , the error probability of the estimator θ^{est} is defined as

$$P\{\Delta(\theta_i^{\text{est}}, \theta_i) \geq \varepsilon\} = \langle s_i^{(\varepsilon, \theta)} \rangle_{D, \theta}^{\text{exp}}. \quad (4.14)$$

We define the expected loss for the squared error.

Definition 32. We call the expected loss of squared error as mean squared error. We denote it as $\Delta_2^{\text{exp}}(\theta_i^{\text{est}}, \theta_i)$.

Now we define the variance of a random variable.

Definition 33. For a random variable $x \in \mathbb{R}$, the variance of the random variable $\sigma(x)$ is defined by

$$\sigma(x) = \langle (x - \langle x \rangle_x^{\text{exp}})^2 \rangle_x^{\text{exp}}. \quad (4.15)$$

For any function $f : \mathbb{R} \rightarrow \mathbb{C}$, we can also define the variance $\sigma_x(f)$ of the function in the random variable x as

$$\sigma_x(f) = \langle |f(x) - \langle f \rangle_x^{\text{exp}}|^2 \rangle_x^{\text{exp}}. \quad (4.16)$$

When the probability distribution depends on the statistical parameter θ , we describe the dependency on the variance as $\sigma_{x, \theta}$.

The mean squared error is related to the variance of a measurement.

Lemma 11. When the expectation value of an element of an estimator is equal to a stochastic parameter $\theta_i = \langle \theta_i^{\text{est}} \rangle_{D, \theta}^{\text{exp}}$, the mean squared error is equal to the variance, namely,

$$\sigma_{D, \theta}(\theta_i^{\text{est}}) = \Delta_2^{\text{exp}}(\theta_i^{\text{est}}). \quad (4.17)$$

This fact is trivially proven by the definitions of the variance and mean squared error. As an important property of the variance, we introduce Chebichev's inequality.

Lemma 12 (Chebichev's inequality). For any random variable $x \in \mathbb{C}$ and a complex function f ,

$$P\left\{|f(x) - \langle f \rangle_x^{\text{exp}}|^2 \geq \frac{\sigma_x(f)}{\varepsilon}\right\} \leq \varepsilon. \quad (4.18)$$

is satisfied.

We skip this proof, since this is shown in standard probability theory textbooks [37]. Please note that $\Delta_2^{\text{exp}}(\theta_i^{\text{est}}, \theta_i)$ is the upper bound for the variance of each element of the estimator θ_i^{est} . For estimation problems, the following corollary which connects the mean squared error and the error probability is useful.

Corollary 2. *When an estimator satisfies $\langle \theta_i^{\text{est}} \rangle_D^{\text{exp}} = \theta_i$, the following formula for the mean squared error and the error probability holds:*

$$P \left\{ |\theta_i - \theta_i^{\text{est}}| \geq \sqrt{\frac{\Delta_2^{\text{exp}}(\theta_i^{\text{est}}, \theta_i)}{\varepsilon}} \right\} \leq \varepsilon. \quad (4.19)$$

In the rest of this section, to estimate an unknown unitary operation, we perform several two-valued measurements and convert the data by a linear estimator. Thus we introduce the following two theorems of a linear estimator for two-valued data.

Theorem 4. *Assume that the parameter of a probability distribution and a linear estimator is given by*

$$\theta_i = \sum_k \langle f_i^{(k)} \rangle_{x,\theta}^{\text{exp}}, \quad \theta_i^{\text{est}} = \sum_k \langle f_i^{(k)} \rangle_{D^{(k)}}^{\text{ave}}. \quad (4.20)$$

Then the expected loss Δ_2 of this estimator satisfies

$$\Delta_2^{\text{exp}}(\theta_i, \theta_i^{\text{est}}) = \sum_k \sigma_{D^{(k)},\theta}(f_i^{(k)}). \quad (4.21)$$

Theorem 5. *Assume that the parameter of a probability distribution and a linear estimator is given by*

$$\theta_i = \sum_k \langle f_i^{(k)} \rangle_{x,\theta}^{\text{exp}}, \quad \theta_i^{\text{est}} = \sum_k \langle f_i^{(k)} \rangle_{D^{(k)}}^{\text{ave}}. \quad (4.22)$$

The expected loss Δ_4 satisfies

$$\Delta_4^{\text{exp}}(\theta_i^{\text{est}}) \leq 3 \left(\Delta_2^{\text{exp}}(\theta_i^{\text{est}}) \right)^2 + 2 \max_l |f_i^{(l)}(a) - f_i^{(l)}(b)|^2 \Delta_2^{\text{exp}}(\theta_i^{\text{est}}). \quad (4.23)$$

To prove these theorems, we show the following two lemmas.

Lemma 13. *Assume that x is a two-valued random variable which takes the value a in probability p_θ and b in $1 - p_\theta$. For any $f : \mathbb{R} \rightarrow \mathbb{C}$, the variance obeys*

$$\sigma_{D,\theta}(f) = \frac{\sigma_{x,\theta}(f)}{M}, \quad (4.24)$$

where $\sigma_{x,\theta}$ is the variance of $f(x)$, which is given as

$$\sigma_{x,\theta}(f) = |f(a) - f(b)|^2 p_\theta(1 - p_\theta), \quad (4.25)$$

and M is the number of data D .

Proof. By definition, the variance of the sample mean can be transformed as

$$\sigma_{D,\theta}(f) = \sum_{k=0}^M p_\theta^k (1-p_\theta)^{M-k} \frac{M!}{k!(M-k)!} \left| \left(f_i(a) \frac{k}{M} - f_i(b) \frac{M-k}{M} \right) - \langle f_i \rangle_\theta^{\text{exp}} \right|^2. \quad (4.26)$$

Since

$$\langle f_i \rangle_{x,\theta}^{\text{exp}} = p_\theta f_i(a) - (1-p_\theta) f_i(b), \quad (4.27)$$

we simplify $\sigma_{D,\theta}(f)$ as

$$\begin{aligned} \sigma_{D,\theta}(f) &= |f(a) - f(b)|^2 \sum_{k=0}^M p_\theta^k (1-p_\theta)^{M-k} \\ &\quad \times \frac{M!}{k!(M-k)!} \left(\frac{k}{M} - p_\theta \right) \left((1-p_\theta) - \frac{M-k}{M} \right). \end{aligned} \quad (4.28)$$

We expand the last two parentheses as

$$\begin{aligned} \sigma_{D,\theta}(f) &= |f(a) - f(b)|^2 \sum_{k=0}^M p_\theta^k (1-p_\theta)^{M-k} \\ &\quad \times \left[\frac{M!}{k!(M-k)!} \frac{k}{M} (1-p_\theta) + \frac{M!}{k!(M-k)!} \frac{(M-k)}{M} p_\theta \right. \\ &\quad \left. - \frac{M!}{k!(M-k)!} p_\theta (1-p_\theta) - \frac{M!}{k!(M-k)!} \frac{k(M-k)}{M^2} \right]. \end{aligned} \quad (4.29)$$

By using ${}_n C_k = n!/k!(n-k)!$, we rewrite this equation as

$$\begin{aligned} \sigma_{D,\theta}(f) &= |f(a) - f(b)|^2 \left[(1-p_\theta) \sum_{k=1}^M {}_{M-1} C_{k-1} \right. \\ &\quad \left. + p_\theta \sum_{k=0}^{M-1} {}_{M-1} C_k - p_\theta (1-p_\theta) \sum_{k=0}^M {}_M C_k - \frac{M-1}{M} \sum_{k=1}^{M-1} {}_{M-2} C_{k-1} \right] p_\theta^k (1-p_\theta)^{M-k}. \end{aligned} \quad (4.30)$$

Now, we factor out $p_\theta(1-p_\theta)$ from the above equation as

$$\begin{aligned} \sigma_{D,\theta}(f) &= |f(a) - f(b)|^2 p_\theta(1-p_\theta) \left[2 \sum_{k=0}^{M-1} {}_{M-1} C_k p_\theta^k (1-p_\theta)^{M-k-1} \right. \\ &\quad \left. - \sum_{k=0}^M {}_M C_k p_\theta^k (1-p_\theta)^{M-k} - \frac{M-1}{M} \sum_{k=0}^{M-2} {}_{M-2} C_k p_\theta^{k-1} (1-p_\theta)^{M-k-1} \right] \end{aligned} \quad (4.31)$$

Because of the binomial theorem, it is transformed as

$$\begin{aligned} \sigma_{D,\theta}(f) &= |f(a) - f(b)|^2 p_\theta(1 - p_\theta) \\ &\times \left[2(p_\theta + (1 - p_\theta))^{M-1} - (p_\theta + (1 - p_\theta))^M - \frac{M-1}{M}(p_\theta + (1 - p_\theta))^{M-2} \right]. \end{aligned} \quad (4.32)$$

Then we obtain

$$\sigma_{D,\theta}(f) = |f(a) - f(b)|^2 \frac{p_\theta(1 - p_\theta)}{M}. \quad (4.33)$$

Therefore, we complete the proof of Lemma 13. \square

Lemma 14. *Assume that x is a two-valued random variable which takes the value a in probability p_θ and b in $1 - p$. For any $f : \mathbb{R} \rightarrow \mathbb{C}$, the following relationship is satisfied:*

$$\sigma_{D,\theta}^{(4)}(f) \leq 3\sigma_{D,\theta}^2(f) + 2|f(a) - f(b)|^2 \sigma_{D,\theta}(f), \quad (4.34)$$

where $\sigma_{D,\theta}^{(4)}(f)$ is

$$\sigma_{D,\theta}^{(4)}(f) = \left\langle \left| \langle f \rangle_D^{\text{ave}} - \langle f \rangle_{x,\theta}^{\text{exp}} \right|^4 \right\rangle_{D,\theta}^{\text{exp}}, \quad (4.35)$$

and M is the number of the data D .

Proof. Similarly to the proof of Lemma 13, we obtain

$$\begin{aligned} \sigma_{D,\theta}^{(4)}(f) &= |f(a) - f(b)|^4 \left[\frac{M^2 + 3M - 6}{M^3} p^2(1 - p)^2 \right. \\ &\quad \left. + \frac{M-1}{M^2} (1 - 2p)p(1 - p) + \frac{1}{M^2} p(1 - p) \right]. \end{aligned} \quad (4.36)$$

We organize this equation as

$$\begin{aligned} \sigma_{D,\theta}^{(4)}(f) &= |f(a) - f(b)|^4 \\ &\times \left[\frac{1}{M} p^2(1 - p)^2 + \frac{3}{M^2} p^2(1 - p)^2 - \frac{6}{M^3} p^2(1 - p)^2 \right. \\ &\quad \left. + \frac{1}{M} (1 - 2p)p(1 - p) + \frac{2p}{M^2} p(1 - p) \right]. \end{aligned} \quad (4.37)$$

Since the third term is negative, erasing this term increases the total value. Taking account of the inequality $1/M^2 \leq 1/M$, we have

$$\sigma_{D,\theta}^{(4)}(f) \leq |f(a) - f(b)|^4 \left[\frac{3}{M^2} p^2(1 - p)^2 + \frac{1}{M} p^2(1 - p)^2 + \frac{1}{M} p(1 - p) \right] \quad (4.38)$$

Since $p^2(1-p)^2 \leq p(1-p)$, then

$$\sigma_{D,\theta}^{(4)}(f) \leq |f(a) - f(b)|^4 \left(\frac{3}{M^2} p^2(1-p)^2 + \frac{2}{M} p(1-p) \right). \quad (4.39)$$

Applying Eq. (4.33) to this inequality, we conclude

$$\sigma_{D,\theta}^{(4)}(f) \leq 3\sigma_{D,\theta}^2(f) + 2|f(a) - f(b)|^2 \sigma_{D,\theta}(f). \quad (4.40)$$

□

The proofs of Theorem 4 and Theorem 5 are given as follows.

Proof of Theorem. 4. By definition, the expected loss can be represented as

$$\Delta_2^{\text{exp}}(\theta_i^{\text{est}}) = \sum_{k,l} \left\langle \left(\langle f_i^{(k)} \rangle_{D^{(k)}}^{\text{ave}} - \langle f_i^{(k)} \rangle_{x,\theta}^{\text{exp}} \right) \left(\langle f_i^{(l)} \rangle_{D^{(l)}}^{\text{ave}} - \langle f_i^{(l)} \rangle_{x,\theta}^{\text{exp}} \right)^* \right\rangle_{D,\theta}^{\text{exp}}. \quad (4.41)$$

Note that for all $k \neq l$,

$$\begin{aligned} & \left\langle \left(\langle f_i^{(k)} \rangle_{D^{(k)}}^{\text{ave}} - \langle f_i^{(k)} \rangle_{x,\theta}^{\text{exp}} \right) \left(\langle f_i^{(l)} \rangle_{D^{(l)}}^{\text{ave}} - \langle f_i^{(l)} \rangle_{x,\theta}^{\text{exp}} \right)^* \right\rangle_{D,\theta}^{\text{exp}} \\ &= \left\langle \left(\langle f_i^{(k)} \rangle_{D^{(k)}}^{\text{ave}} - \langle f_i^{(k)} \rangle_{x,\theta}^{\text{exp}} \right) \right\rangle_{D^{(k)},\theta}^{\text{exp}} \left\langle \left(\langle f_i^{(l)} \rangle_{D^{(l)}}^{\text{ave}} - \langle f_i^{(l)} \rangle_{x,\theta}^{\text{exp}} \right)^* \right\rangle_{D^{(l)},\theta}^{\text{exp}} = 0 \end{aligned} \quad (4.42)$$

is satisfied where x_k and x_l are statistically independent. Then we can simplify Eq.(4.45) as

$$\Delta_2^{\text{exp}}(\theta_i) = \sum_k \left\langle \left| \langle f_i^{(k)} \rangle_{D^{(k)}}^{\text{ave}} - \langle f_i^{(k)} \rangle_{x,\theta}^{\text{exp}} \right|^2 \right\rangle_{D^{(k)},\theta}^{\text{exp}}. \quad (4.43)$$

Each term in the summation part in the right-hand side is $\sigma_{\theta}^{M^{(k)}}(f_i^{(k)})$. Thus we conclude the theorem. □

Proof of Theorem5. By definition, $\Delta_4^{\text{exp}}(\theta^{\text{exp}})$ is decomposed as

$$\begin{aligned} \Delta_4^{\text{exp}}(\theta_i^{\text{est}}) &= \sum_{k,l,m,n} \left\langle \left(\langle f_i^{(k)} \rangle_{D^{(k)}}^{\text{ave}} - \langle f_i^{(k)} \rangle_{x,\theta}^{\text{exp}} \right) \left(\langle f_i^{(l)} \rangle_{D^{(l)}}^{\text{ave}} - \langle f_i^{(l)} \rangle_{x,\theta}^{\text{exp}} \right)^* \right. \\ & \quad \left. \left(\langle f_i^{(m)} \rangle_{D^{(m)}}^{\text{ave}} - \langle f_i^{(m)} \rangle_{x,\theta}^{\text{exp}} \right) \left(\langle f_i^{(n)} \rangle_{D^{(n)}}^{\text{ave}} - \langle f_i^{(n)} \rangle_{x,\theta}^{\text{exp}} \right)^* \right\rangle_{D,\theta}^{\text{exp}}. \end{aligned} \quad (4.44)$$

Using the condition $\left\langle \langle f_i \rangle_{D^{(k)}}^{\text{ave}} - \langle f_i \rangle_{D^{(k)}}^{\text{exp}} \right\rangle_{D,\theta}^{\text{exp}} = 0$, only certain terms survive, and we obtain

$$\begin{aligned} \Delta_4^{\text{exp}}(\theta_i^{\text{est}}) &= \sum_k \left\langle \left| \langle f_i^{(k)} \rangle_{D^{(k)}}^{\text{ave}} - \langle f_i^{(k)} \rangle_{x,\theta}^{\text{exp}} \right|^4 \right\rangle_{D,\theta}^{\text{exp}} \\ &+ 2 \sum_{k \neq l} \left\langle \left| \langle f_i^{(k)} \rangle_{D^{(k)}}^{\text{ave}} - \langle f_i^{(k)} \rangle_{x,\theta}^{\text{exp}} \right|^2 \right\rangle_{D,\theta}^{\text{exp}} \left\langle \left| \langle f_i^{(l)} \rangle_{D^{(l)}}^{\text{ave}} - \langle f_i^{(l)} \rangle_{x,\theta}^{\text{exp}} \right|^2 \right\rangle_{D,\theta}^{\text{exp}} \\ &+ \sum_{k \neq l} \left\langle \left(\langle f_i^{(k)} \rangle_{D^{(k)}}^{\text{ave}} - \langle f_i^{(k)} \rangle_{x,\theta}^{\text{exp}} \right)^2 \right\rangle_{D,\theta}^{\text{exp}} \left\langle \left(\langle f_i^{(l)} \rangle_{D^{(l)}}^{\text{ave}} - \langle f_i^{(l)} \rangle_{x,\theta}^{\text{exp}} \right)^* \right\rangle_{D,\theta}^{\text{exp}}. \end{aligned} \quad (4.45)$$

Since

$$\left| \left\langle \left(\langle f_i^{(k)} \rangle_{D^{(k)}}^{\text{ave}} - \langle f_i^{(k)} \rangle_{x,\theta}^{\text{exp}} \right)^2 \right\rangle \right| \leq \left\langle \left| \langle f_i^{(k)} \rangle_{D^{(k)}}^{\text{ave}} - \langle f_i^{(k)} \rangle_{x,\theta}^{\text{exp}} \right|^2 \right\rangle, \quad (4.46)$$

then we have

$$\begin{aligned} \Delta_4^{\text{exp}}(\theta_i^{\text{est}}) &\leq \sum_k \left\langle \left| \langle f_i^{(k)} \rangle_{D^{(k)}}^{\text{ave}} - \langle f_i^{(k)} \rangle_{x,\theta}^{\text{exp}} \right|^4 \right\rangle_{D,\theta}^{\text{exp}} \\ &\quad + 3 \sum_{k \neq l} \left\langle \left| \langle f_i^{(k)} \rangle_{D^{(k)}}^{\text{ave}} - \langle f_i^{(k)} \rangle_{x,\theta}^{\text{exp}} \right|^2 \right\rangle_{D,\theta}^{\text{exp}} \left\langle \left| \langle f_i^{(l)} \rangle_{D^{(l)}}^{\text{ave}} - \langle f_i^{(l)} \rangle_{x,\theta}^{\text{exp}} \right|^2 \right\rangle_{D,\theta}^{\text{exp}}. \end{aligned} \quad (4.47)$$

Using Lemma 13 for the first term and Lemma 14 for the second, we obtain

$$\begin{aligned} \Delta_4^{\text{exp}}(\theta_i^{\text{est}}) &\leq 3 \sum_k \sigma_{D^{(k)},\theta}(f_i^{(k)}) \sum_l \sigma_{D^{(l)},\theta}(f_i^{(l)}) \\ &\quad + 2 \max_l \left| f_i^{(l)}(a) - f_i^{(l)}(b) \right|^2 \sum_k \sigma_{D^{(k)},\theta}(f_i^{(k)}). \end{aligned} \quad (4.48)$$

According to Theorem 5, we conclude that

$$\Delta_4^{\text{exp}}(\theta_i^{\text{est}}) \leq 3 \left(\Delta_2^{\text{exp}}(\theta_i^{\text{est}}) \right)^2 + 2 \max_l \left| f_i^{(l)}(a) - f_i^{(l)}(b) \right|^2 \Delta_2^{\text{exp}}(\theta_i^{\text{est}}). \quad (4.49)$$

□

4.3 Identifying unitary dynamics

We have introduced a straight forward way to identify an unknown unitary dynamics U up to its global phase. In the following, we limit the quantum system to a q -qubits system $(\mathbb{C}^2)^{\otimes q}$. We denote the dimension of this system as $d = 2^q$.

We define a vector \mathbf{n} in a vector space $(\mathbb{Z}_2)^{\otimes q}$ for any natural number $0 \leq n \leq d - 1$. Let $\{\mathbf{e}_k\}$ be an orthogonal basis, and \mathbf{n} is defined as

$$\mathbf{n} = \sum_k n_k \mathbf{e}_k \quad (4.50)$$

where $n_k \in \mathbb{Z}_2$ is the k -th digit number of n in the binary representation defined as $n = \sum_{k=0}^{q-1} 2^k n_k$. The sum of vectors in the vector space is defined by

$$\mathbf{n} + \mathbf{m} = \sum_k l_k \mathbf{e}_k, \quad (4.51)$$

where

$$l_k = n_k + m_k \pmod{2}. \quad (4.52)$$

We construct a basis $\{|\mathbf{n}\rangle | 0 \leq n \leq d-1\}$ in $(\mathbb{C}^2)^{\otimes q}$ each of which is defined as

$$|\mathbf{n}\rangle := \bigotimes_{k=1}^q |n_k\rangle = |n_1 n_2 \dots n_q\rangle. \quad (4.53)$$

If $\langle \mathbf{0} | U | \mathbf{0} \rangle \neq 0$, all the elements of unitary U are perfectly determined by a matrix Θ up to the global phase where the n, m element of Θ is defined by

$$\Theta_{nm} = \langle \mathbf{n} | U | \mathbf{m} \rangle \langle \mathbf{0} | U^\dagger | \mathbf{0} \rangle. \quad (4.54)$$

We define the generalized Pauli matrices $X_i^{(j)}$ on this Hilbert space for any pair of integers $0 \leq i \leq d-1$ and, $0 \leq j \leq d-1$ as

$$X_j^{(i)} = \bigotimes_{k=1}^q X_{j_k}^{(i_k)}, \quad (4.55)$$

where $i_k, j_k = 0, 1$ are also defined as the k -th digit numbers defined by

$$i = \sum_{k=1}^q 2^{k-1} i_k, \quad j = \sum_{k=1}^q 2^{k-1} j_k. \quad (4.56)$$

$X_i^{(j)}$ is a Pauli matrix on a single qubit defined as

$$X_0^{(0)} = |0\rangle\langle 0| + |1\rangle\langle 1|, \quad (4.57)$$

$$X_0^{(1)} = |0\rangle\langle 0| - |1\rangle\langle 1|, \quad (4.58)$$

$$X_1^{(0)} = |0\rangle\langle 1| + |1\rangle\langle 0|, \quad (4.59)$$

$$X_1^{(1)} = i(|0\rangle\langle 1| - |1\rangle\langle 0|). \quad (4.60)$$

We define operators s_0, s_1 on a 1-qubit Hilbert space by

$$s_0 = |0\rangle\langle 0|, \quad (4.61)$$

$$s_1 = |0\rangle\langle 1|. \quad (4.62)$$

For a q -qubit system, we also define an operator.

$$S_n := |\mathbf{0}\rangle\langle \mathbf{n}|. \quad (4.63)$$

Note that

$$\langle \psi | S_n | \phi \rangle = \langle \mathbf{n} | \phi \rangle \langle \psi | \mathbf{0} \rangle. \quad (4.64)$$

Due to Eqs. (4.57)–(4.60), s_i is written by

$$s_j = \frac{X_j^{(0)} + (-i)^j X_j^{(1)}}{2}. \quad (4.65)$$

On the other hand, S_n can be represented in the product of s_j as

$$S_n = \bigotimes_{k=0}^{q-1} s_{n_k} \quad (4.66)$$

Substituting Eq. (4.65) into Eq. (4.66), we obtain

$$S_n = \frac{1}{d} \sum_{i=0}^{d-1} (-i)^{n \cdot i} X_n^{(i)}. \quad (4.67)$$

For index $m \neq 0$, we associate four vectors by

$$|\mathbf{m}, 0\rangle = \frac{1}{\sqrt{2}} (|\mathbf{0}\rangle + |\mathbf{m}\rangle), \quad (4.68)$$

$$|\mathbf{m}, 1\rangle = \frac{1}{\sqrt{2}} (|\mathbf{0}\rangle + i|\mathbf{m}\rangle), \quad (4.69)$$

$$|\mathbf{m}, 2\rangle = \frac{1}{\sqrt{2}} (|\mathbf{0}\rangle - |\mathbf{m}\rangle), \quad (4.70)$$

$$|\mathbf{m}, 3\rangle = \frac{1}{\sqrt{2}} (|\mathbf{0}\rangle - i|\mathbf{m}\rangle). \quad (4.71)$$

For these vectors,

$$\frac{1}{2} \sum_{s=0}^3 (-i)^s \langle \mathbf{m}, s | A | \mathbf{m}, s \rangle = \langle \mathbf{0} | A | \mathbf{m} \rangle, \quad (4.72)$$

is satisfied, where A is an operator on a Hilbert space $(\mathbb{C}^2)^{\otimes q}$.

We define random variables $x_{nm}^{(i,s)}$ as the outcome of the following measurement process. We initially prepare a state $|\mathbf{m}, s\rangle$. Next we apply the unknown unitary U on the state. Then we perform a measurement of observable $X_n^{(i)}$ on the state. The expectation value of the measurement is given by.

$$\langle x_{nm}^{(i,s)} \rangle_{\Theta}^{\text{exp}} = \langle \mathbf{m}, s | U^\dagger X_n^{(i)} U | \mathbf{m}, s \rangle \quad (4.73)$$

We define other random variables $x_{n0}^{(i)}$ for the outcome of a measurement $X_n^{(i)}$ on the state $U|\mathbf{0}\rangle$, which satisfies

$$\langle x_{n0}^{(i)} \rangle_{\Theta}^{\text{exp}} = \langle \mathbf{0} | U^\dagger X_n^{(i)} U | \mathbf{0} \rangle. \quad (4.74)$$

According to Eqs. (4.64),(4.67),(4.72) and (4.73), we conclude that any Θ_{nm} is given as

$$\Theta_{nm} = \frac{1}{2d} \sum_{i=0}^{d-1} \sum_{s=0}^3 (-i)^s (-i)^{n \cdot i} \langle x_{nm}^{(i,s)} \rangle_{\Theta}^{\text{exp}}. \quad (4.75)$$

We can also derive

$$\Theta_{n0} = \frac{1}{d} \sum_{i=0}^{d-1} (-i)^{n \cdot i} \langle x_{n0}^{(i)} \rangle_{\Theta}^{\text{exp}}. \quad (4.76)$$

Assume that we iterate each measurement on each state M times. Let us define each datum as $D_{nm}^{(i,s)}$. We also define

$$D = \{D_{nm}^{(i,s)} | 0 \leq m \leq d-1, 0 \leq n \leq d-1, 0 \leq i \leq d-1, 0 \leq s \leq 3\}. \quad (4.77)$$

We define the linear estimator of each element of the parameter Θ_{nm} as for $m \neq 0$,

$$\Theta_{nm}^{\text{est}}(D) = \frac{1}{2d} \sum_{i=0}^{d-1} \sum_{s=0}^3 (-i)^s (-i)^{n \cdot i} \langle x_{nm}^{(i,s)} \rangle_{D_{nm}^{(i,s)}}^{\text{ave}}, \quad (4.78)$$

and for $m = 0$,

$$\Theta_{n0}^{\text{est}} = \frac{1}{d} \sum_{i=0}^{d-1} (-i)^{n \cdot i} \langle x_{n0}^{(i)} \rangle_{D_{n0}^{(i)}}^{\text{ave}}. \quad (4.79)$$

For this linear estimator, the following theorem is satisfied.

Theorem 6. *The estimator Θ^{est} defined by Eq. (4.78) and (4.79) has the Θ -independent upper and lower bound for its loss functions given as*

$$\Delta_2^{\text{exp}}(\Theta_{nm}, \Theta_{nm}^{\text{est}}) \leq \frac{1}{dM} \quad (n + m \neq 0), \quad (4.80)$$

$$\Delta_2^{\text{exp}}(\Theta_{00}, \Theta_{00}^{\text{est}}) \leq \frac{1}{dM}. \quad (4.81)$$

Proof. Since each measurement has a two-valued outcome, according to Theorem 4, the expected loss is given as for $m \neq 0$

$$\Delta_2^{\text{exp}}(\Theta_{nm}, \Theta_{nm}^{\text{est}}) = \frac{1}{4d^2} \sum_{s=0}^3 \frac{\sum_{i=0}^{d-1} \sigma_{nm}^{(i,s)}}{M}, \quad (4.82)$$

and for $m = 0$,

$$\Delta_2^{\text{exp}}(\Theta_{n0}, \Theta_{n0}^{\text{est}}) = \frac{1}{d^2} \frac{\sum_{i=0}^{d-1} \sigma_{n0}^{(i)}}{M}. \quad (4.83)$$

$\sigma_{nm}^{(i,s)}$ is the variance of the random variable $x_{nm}^{(i,s)}$ and $\sigma_{n0}^{(i)}$ is the one of $x_{n0}^{(i)}$. Since $x_{nm}^{(i,s)} = \pm 1$ and $x_{n0}^{(i)} = \pm 1$, we have

$$\sigma_{nm}^{(i,s)} = 1 - \left(\langle x_{nm}^{(i,s)} \rangle_{\Theta}^{\text{exp}} \right)^2, \quad (4.84)$$

$$\sigma_{n0}^{(i)} = 1 - \left(\langle x_{n0}^{(i)} \rangle_{\Theta}^{\text{exp}} \right)^2. \quad (4.85)$$

Substituting Eq. (4.84) in Eq. (4.82), the upper bound of the expected loss is evaluated as

$$\Delta_2^{\text{exp}}(\Theta_{nm}, \Theta_{nm}^{\text{est}}) \leq \frac{1}{dM}. \quad (4.86)$$

With the similar discussion, we derive

$$\Delta_2^{\text{exp}}(\Theta_{00}, \Theta_{00}^{\text{est}}) \leq \frac{1}{dM}. \quad (4.87)$$

□

We introduce several properties of a matrix V defined as

$$V = \Theta^{\text{est}} - \Theta, \quad (4.88)$$

The following evaluation takes an important role in implementation of the projective measurement of energy.

Theorem 7. For any vector $|\phi\rangle \in (\mathbb{C}^2)^{\otimes q}$,

$$\langle \langle \phi | |V|^2 | \phi \rangle \rangle_{D, \Theta}^{\text{exp}} \leq \frac{1}{M}. \quad (4.89)$$

Theorem 8. For any vector $|\phi\rangle \in (\mathbb{C}^2)^{\otimes q}$,

$$\langle \langle \phi | |V|^2 | \phi \rangle \rangle_{D, \Theta}^{\text{exp}} \leq \frac{12}{M} + \frac{9}{M^2}. \quad (4.90)$$

Before proving these two theorems, we introduce a decomposition of the vector $|\phi\rangle \in (\mathbb{C}^2)^{\otimes q}$ in computational basis denoted by.

$$|\phi\rangle = \sum_n C_n |\mathbf{n}\rangle. \quad (4.91)$$

Theorem. 7. $\langle \phi | |V|^2 | \phi \rangle$ is calculated as

$$\langle \phi | |V|^2 | \phi \rangle = \sum_{nm} \sum_k V_{nk} V_{mk}^* C_n^* C_m. \quad (4.92)$$

For $n \neq m$,

$$\langle V_{nk}^* V_{mk} \rangle_{D, \Theta}^{\text{exp}} = 0 \quad (4.93)$$

is satisfied since the probability distribution for each element of the estimator is independent and the expectation value is set to zero. On the other hand, by definition, the squared absolute value of each element of V statistically behaves as

$$\langle |V_{nm}|^2 \rangle_{D, \Theta}^{\text{exp}} = \Delta_2^{\text{exp}}(\Theta_{nm}^{\text{ext}}, \Theta_{nm}). \quad (4.94)$$

Then

$$\langle \langle \phi | |V|^2 | \phi \rangle \rangle_{D, \Theta}^{\text{exp}} = \sum_n \sum_k \Delta_2^{\text{exp}}(\Theta_{nk}^{\text{ext}}, \Theta_{nk}) |C_n|^2. \quad (4.95)$$

Due to the upper bound given in Theorem 6, we have

$$\langle \langle \phi | |V|^2 | \phi \rangle \rangle_{D, \Theta}^{\text{exp}} \leq \sum_n \sum_k \frac{1}{dM} |C_n|^2 \quad (4.96)$$

$$= \frac{1}{M} \sum_n |C_n|^2 = \frac{1}{M} \quad (4.97)$$

□

Proof of Theorem 8. $|\langle \phi | |V|^2 | \phi \rangle|^2$ is given by

$$|\langle \phi | |V|^2 | \phi \rangle|^2 = \sum_{nm} \sum_{ab} \sum_{kl} V_{nk} V_{mk}^* V_{al} V_{bl} C_n^* C_m C_a C_b^*. \quad (4.98)$$

Similarly to the relationship in Eq. (4.93), even though more multiplications of V_{nm} appear, when a combination of indices nm appears only once in a term, the term becomes zero. Then only certain terms in the equation survive after taking average in probability,

$$\begin{aligned} \langle |\langle \phi | |V|^2 | \phi \rangle|^2 \rangle_{D, \Theta}^{\text{exp}} &= \sum_{na} \sum_{kl} \langle |V_{nk}|^2 |V_{al}|^2 \rangle_{D, \Theta}^{\text{exp}} |C_n|^2 |C_a|^2 \\ &+ \sum_{nm} \sum_k \langle |V_{nk}|^2 |V_{mk}|^2 \rangle_{D, \Theta}^{\text{exp}} |C_n|^2 |C_m|^2 \\ &+ \sum_{nm} \sum_k \langle V_{nk}^2 V_{mk}^{*2} \rangle_{D, \Theta}^{\text{exp}} C_n^2 C_m^{*2} \end{aligned} \quad (4.99)$$

Taking the absolute value for the factors in the last term of the above equation, we obtain

$$\begin{aligned} \langle |\langle \phi | |V|^2 | \phi \rangle|^2 \rangle_{D, \Theta}^{\text{exp}} &\leq \sum_{na} \sum_{kl} \langle |V_{nk}|^2 |V_{al}|^2 \rangle_{D, \Theta}^{\text{exp}} |C_n|^2 |C_a|^2 \\ &+ 2 \sum_{nm} \sum_k \langle |V_{nk}|^2 |V_{mk}|^2 \rangle_{D, \Theta}^{\text{exp}} |C_n|^2 |C_m|^2. \end{aligned} \quad (4.100)$$

According to Eq. (4.94) and the relationship

$$\langle |V_{nm}|^4 \rangle_{D, \Theta}^{\text{exp}} = \Delta_4^{\text{exp}}(\Theta_{nm}^{\text{est}}, \Theta_{nm}), \quad (4.101)$$

the value of interest is bounded as

$$\begin{aligned} \left\langle \left| \langle \phi | |V|^2 | \phi \rangle \right|^2 \right\rangle_{D, \Theta}^{\text{exp}} &\leq \sum_{na} \sum_{kl} \Delta_2^{\text{exp}}(\Theta_{nk}^{\text{exp}}) \Delta_2^{\text{exp}}(\Theta_{al}^{\text{exp}}) |C_n|^2 |C_a|^2 \\ &\quad + 2 \sum_{nm} \sum_k \Delta_2^{\text{exp}}(\Theta_{nk}^{\text{exp}}) \Delta_2^{\text{exp}}(\Theta_{mk}^{\text{exp}}) |C_n|^2 |C_m|^2 \\ &\quad + 3 \sum_n \sum_k \left(\Delta_4^{\text{exp}}(\Theta_{nk}^{\text{est}}) - \left(\Delta_2^{\text{exp}}(\Theta_{nk}^{\text{exp}}) \right)^2 \right) |C_n|^4. \end{aligned} \quad (4.102)$$

Applying Theorem 5 for our setting, we achieve

$$\Delta_4^{\text{exp}}(\Theta_{nm}^{\text{est}}) \leq 3 \left(\Delta_2^{\text{exp}}(\Theta_{nm}^{\text{est}}) \right)^2 + \frac{4}{d^2} \Delta_2^{\text{exp}}(\Theta^{\text{est}}). \quad (4.103)$$

Substitute the above inequality and the bound of $\Delta_2^{\text{est}}(\Theta_{nm}^{\text{est}})$ mentioned before

$$\left\langle \left| \langle \phi | |V|^2 | \phi \rangle \right|^2 \right\rangle_{D, \Theta}^{\text{exp}} \leq \frac{1}{M^2} + \frac{2}{dM^2} + \frac{1}{d^2} \left(\frac{12}{M} + \frac{6}{dM^2} \right) \sum_n |C_n|^4. \quad (4.104)$$

Because $|C_n| \leq 1$,

$$\sum_n |C_n|^4 \leq \sum_n |C_n|^2 = 1. \quad (4.105)$$

Then

$$\left\langle \left| \langle \phi | |V|^2 | \phi \rangle \right|^2 \right\rangle_{D, \Theta}^{\text{exp}} \leq \frac{1}{M^2} + \frac{2}{dM^2} + \frac{12}{d^2 M} + \frac{6}{d^3 M^2}. \quad (4.106)$$

Substitute $1/d \leq 1$ into (4.106), we obtain

$$\left\langle \left| \langle \phi | |V|^2 | \phi \rangle \right|^2 \right\rangle_{D, \Theta}^{\text{exp}} \leq \frac{12}{M} + \frac{9}{M^2}. \quad (4.107)$$

□

4.4 Implementing projective measurement of energy

4.4.1 Implementing projective measurement of energy

We propose an implementation method of the projective measurement of energy using the estimated parameter Θ^{est} , when the unitary operation is given by the dynamics of an unknown Hamiltonian H with duration time t . We take the Hamiltonian H as it absorbs the complex factor (global phase) of $\langle \mathbf{0} | U | \mathbf{0} \rangle$, among the arbitrariness for choosing the base-point of the energy eigenvalue, and denote

$$\Theta = \sum_{k \in Y} c e^{-iE_k t} P_k, \quad P_k = \sum_{\lambda \in Z_i} |E_k^\lambda\rangle \langle E_k^\lambda|, \quad (4.108)$$

where $c = |\langle \mathbf{0} | U | \mathbf{0} \rangle|$. We also denote the diagonalization of H as

$$H = \sum_{i \in Y} E_i P_i, \quad P_i = \sum_{\lambda \in Z_i} |E_i^\lambda\rangle \langle E_i^\lambda|. \quad (4.109)$$

We assume a bound of the maximum energy difference Δ_{\max} (the largest eigenvalue minus the smallest eigenvalue) of H is known. We take the duration time of the Hamiltonian dynamics t satisfying

$$\Delta_{\max} t < \pi/4. \quad (4.110)$$

Under this condition, the constant c in Θ is not zero. It is proven as follows. Since $\langle \mathbf{0} | U | \mathbf{0} \rangle$ is expanded as

$$\langle \mathbf{0} | U | \mathbf{0} \rangle = \sum_i |\langle \mathbf{0} | E_i^\lambda \rangle|^2 e^{-iE_i t}, \quad (4.111)$$

then

$$\begin{aligned} |\langle \mathbf{0} | U | \mathbf{0} \rangle|^2 &= \sum_{i,j \in Y} \sum_{\lambda \in Z_i, \mu \in Z_j} |\langle \mathbf{0} | E_i^\lambda \rangle|^2 |\langle \mathbf{0} | E_j^\mu \rangle|^2 e^{-i(E_i - E_j)t} \\ &= \sum_{i,j \in Y} \sum_{\lambda \in Z_i, \mu \in Z_j} |\langle \mathbf{0} | E_i^\lambda \rangle|^2 |\langle \mathbf{0} | E_j^\mu \rangle|^2 \cos(E_i - E_j)t. \\ &\geq \sum_{i,j \in Y} \sum_{\lambda \in Z_i, \mu \in Z_j} |\langle \mathbf{0} | E_i^\lambda \rangle|^2 |\langle \mathbf{0} | E_j^\mu \rangle|^2 \cos \Delta_{\max} t, \\ &= \sum_{i,j \in Y} \sum_{\lambda \in Z_i, \mu \in Z_j} |\langle \mathbf{0} | E_i^\lambda \rangle|^2 |\langle \mathbf{0} | E_j^\mu \rangle|^2 \cos \pi/4, \\ &= \cos \pi/4 = \frac{1}{\sqrt{2}}. \end{aligned} \quad (4.112)$$

For simplicity, we impose a condition that the mean value of the Hamiltonian is zero, namely,

$$\frac{1}{d} \sum_{i \in Y} \sum_{\lambda \in Z_i} d_i^\lambda E_i = 0, \quad d_i^\lambda = \text{Tr} [P_i^\lambda] \quad (4.113)$$

Under this condition, each eigenvalue of H satisfies

$$E_i t \in \left[-\frac{\pi}{4}, \frac{\pi}{4} \right]. \quad (4.114)$$

Note that the following arguments are still valid, even when the mean value is not zero. If the mean value is given by e , we just replace the condition of each eigenvalue to

$$E_i t \in \left[-\frac{\pi}{4} + e, \frac{\pi}{4} + e \right]. \quad (4.115)$$

Unfortunately, the linear estimator $\Theta^{\text{est}}(D)$ which we defined in the previous section is expected to estimate non-normal matrices in typical cases since the set of normal matrices is the zero set in the linear space of operators, whereas the expectation value of the estimator Θ^{est} introduced in Sec. 4.3 is a normal matrix Θ . Returning such an *unphysical* outcome is known to be the disadvantage of the linear estimator in general. A non-normal matrix does not have eigenvectors and eigenvalues, which is necessary to identify for implementing projective measurement of energy. For this purpose, we have to deform the obtained matrix into a normal matrix.

In the followings, we impose an assumption that there exist an estimator including a deformation which does not change the probability distribution on each matrix element. We also assume the deformation process guarantees the regularity of the matrix, which is a loose assumption since the set of non-regular matrix is the zero set in the matrix space.

Under these assumptions, we decompose the matrix as

$$\Theta^{\text{est}} = \sum_{k \in X, \alpha \in W} c_{k,\alpha} e^{i\varphi_k} \tilde{P}_{k;\alpha}, \quad \tilde{P}_{k;\alpha} = \sum_{\lambda \in R_{i,\alpha}} |\tilde{E}_{k;\alpha}^\lambda\rangle \langle \tilde{E}_{k;\alpha}^\lambda|, \quad (4.116)$$

where $c_{k,\alpha}$ is a positive number and $e^{i\varphi_k}$ is the absolute value denoting the complex factor of the eigenvalue of Θ^{est} .

According to the estimated matrix Θ^{est} , we assign an estimated energy \tilde{E}_i for each vector $|\tilde{E}_i^\lambda\rangle$ according to each eigenvalue $c_i e^{i\varphi_i}$ of Θ^{est} . As Eq. (4.108), the value of energy is reflected in the complex factor of the eigenvalue. Then intuitively, the energy eigenvalue is determined by the imaginary part of the logarithm of the eigenvalue $c_i e^{i\varphi_i}$. However there is arbitrariness in choosing a branch of the logarithm function. When we know the mean value of the energy is 0, it is reasonable that we take the branch of the logarithm function as a half-line represented as $|z| > 0, \arg z = \pi$. However, we do not know the description of the Hamiltonian beforehand. Thus, we introduce the following logarithm function.

Definition 34. For a normal, regular matrix Θ^{est} having eigenvalues $c_i e^{i\varphi_i}$, we define the primal value of the phase φ_i as $\varphi_i \in [-\pi, \pi]$. We define a complex function Log as it satisfies

$$\alpha = e^{\text{Log}\alpha}, \quad \alpha \in \mathbb{C}, \quad (4.117)$$

and

$$-\pi \leq \left(\text{ImLog}\alpha - \sum_i \frac{\varphi_i}{d} \right) \leq \pi. \quad (4.118)$$

We call this function as a logarithm function for Θ^{est} .

Definition 35. We denote the branch cut of Log as the solution of the equation $\arg z = \varphi_\Theta$ by using a real number $\varphi_\Theta \in [-\pi, \pi]$.

In other words, the function Log is the logarithm function whose branch cut exists on the half-line determined by the solution of the equation $\arg z = \sum_i \varphi_i/d + \pi$. This logarithm function satisfies the following theorem.

Theorem 9. Assume that an estimator Θ^{est} for the parameter Θ satisfies the conditions Eqs. (4.80),(4.81) and the conditions of normality and regularity. We also assume the matrix Θ is determined by a Hamiltonian H as Eqs. (4.108),(4.109) and (4.113), and parameter t satisfies $\Delta_{\max} t < \pi/4$. Then

$$P\{\varphi_\Theta \in [-\pi/2, \pi/2]\} \leq 16d \left(\frac{12}{M} + \frac{9}{M^2} \right). \quad (4.119)$$

Proof. We denote the probability of achieving $\varphi_\Theta \notin [-\pi/2, \pi/2]$ as

$$P\{\varphi_\Theta \notin [-\pi/2, \pi/2]\}. \quad (4.120)$$

Since φ_Θ is given as $\sum_i \varphi_i/d \pm \pi$, when all of φ_i satisfy $\varphi_i \in [-\pi/2, \pi/2]$, φ_Θ is not in the section $[-\pi/2, \pi/2]$. Then, we can bound the probability by that of having at least one index i satisfying $\varphi_i \notin [-\pi/2, \pi/2]$. Thus

$$P\{\varphi_\Theta \notin [-\pi/2, \pi/2]\} \leq P\{\exists i, \varphi_i \notin [-\pi/2, \pi/2]\}. \quad (4.121)$$

Now we decompose an eigenvector of Θ in the ones of Θ^{est} , and we denote

$$|E_i^\lambda\rangle = \sum_{j \in X} \sum_{\alpha \in W_i, \mu \in R_i} v_{ij;\alpha}^{(\lambda\mu)} |\tilde{E}_{j;\alpha}^\mu\rangle. \quad (4.122)$$

We define a matrix V given by Eq. (4.88) and substitute Eq. (4.122) into Eq. (4.147).

$$V|E_i^\lambda\rangle = \sum_{j \in X} \sum_{\alpha \in W_i, \mu \in R_i} \tilde{v}_{ij;\alpha}^{\lambda\mu} (c_{i;\alpha} e^{i\varphi_i} - c e^{-iE_j t}) |\tilde{E}_{j;\alpha}^\mu\rangle \quad (4.123)$$

We define the value Y_i^λ as

$$Y_i^\lambda = \langle E_i^\lambda | |V|^2 |E_i^\lambda\rangle. \quad (4.124)$$

Due to Eq. (4.123), Y_i can be represented as

$$Y_i^\lambda = \sum_{j \in X} \sum_{\alpha \in W_i, \mu \in R_i} \left| \tilde{v}_{ij;\alpha}^{\lambda\mu} \right|^2 (c^2 + c_{j;\alpha}^2 - 2cc_{j;\alpha} \cos(E_j t + \varphi_j)). \quad (4.125)$$

Assume that $\varphi_i \notin [-\pi/2, \pi/2]$. Since E_i satisfies the condition of Eq. (4.115), the cosine function is bounded as

$$\cos(E_j t + \varphi_j) \leq \frac{1}{\sqrt{2}}. \quad (4.126)$$

Substitute this inequality into Eq. (4.125), we obtain

$$Y_i^\lambda \geq (c^2 + c_{j;\alpha}^2 - \sqrt{2}cc_{j;\alpha}). \quad (4.127)$$

Since the right-hand side of this inequality is equal to $(c-c_i)^2 + c^2/2$ and $c \geq 1/\sqrt{2}$ according to Eq. (4.112), then

$$Y_i^\lambda \geq \frac{1}{4}. \quad (4.128)$$

Thus we can conclude that satisfying (4.128) is the necessary condition for being $\varphi_\Theta \notin [-\pi/2, \pi/2]$. Therefore

$$P\{\exists i, \varphi_i \notin [-\pi/2, \pi/2]\} \leq P\left\{\exists i, \lambda, Y_i^\lambda \geq \frac{1}{4}\right\}. \quad (4.129)$$

The values Y_i for indices i are not statistically independent of each other. Then we decompose the probability of achieving at least one Y_i equal to or larger than $1/4$ as

$$P\left\{\exists i, \lambda, Y_i^\lambda \geq \frac{1}{4}\right\} = \sum_{i \in Y} \sum_{\alpha \in Z_i} P\left\{Y_i^\lambda \geq \frac{1}{4}\right\} - \sum_{k=2}^d k \sum_{\substack{i_1, \dots, i_k \in Y \\ \lambda_1 \in Z_{i_1}, \dots, \lambda_k \in Z_{i_k}}} P\left\{Y_{i_1}^{\lambda_1}, \dots, Y_{i_k}^{\lambda_k} \geq \frac{1}{4}\right\}. \quad (4.130)$$

The second term of Eq. (4.130) cancels the counted events. Because of the positivity of the probability, we have

$$P\left\{\exists i, \lambda, Y_i^\lambda \geq \frac{1}{4}\right\} \leq \sum_{i \in Y} \sum_{\alpha \in Z_i} P\left\{Y_i^\lambda \geq \frac{1}{4}\right\}. \quad (4.131)$$

Since the left side of Eq. (4.89) is the expectation value of Y_i^2 , the variance of Y_i is bounded as

$$\begin{aligned} \sigma(Y_i^\lambda) &= \left\langle (Y_i^\lambda)^2 \right\rangle_{D, \Theta}^{\text{exp}} - \left(\left\langle Y_i^\lambda \right\rangle_{D, \Theta}^{\text{exp}} \right)^2 \\ &\leq \left\langle (Y_i^\lambda)^2 \right\rangle_{D, \Theta}^{\text{exp}} \\ &= \left\langle | \langle E_i^\lambda | |V|^2 | E_i^\lambda \rangle |^2 \right\rangle_{D, \Theta}^{\text{exp}} \\ &\leq \left(\frac{12}{M} + \frac{9}{M^2} \right). \end{aligned} \quad (4.132)$$

Using the Chebichev's inequality (Lemma 12) for $Y_i^{(\lambda)}$, we achieve

$$P\left\{Y_i^\lambda \geq \frac{1}{4}\right\} \leq 16\sigma(Y_i^\lambda). \quad (4.133)$$

Therefore according to Eq. (4.132), we achieve a similar bound from the above inequality (4.133), namely,

$$P \left\{ Y_i^\lambda \geq \frac{1}{4} \right\} \leq 16 \left(\frac{12}{M} + \frac{9}{M^2} \right). \quad (4.134)$$

Summarizing Eqs. (4.121),(4.156),(4.157) and (4.134), we reach our goal at last, namely,

$$P \{ \varphi_\Theta \in [-\pi/2, \pi/2] \} \leq 16d \left(\frac{12}{M} + \frac{9}{M^2} \right). \quad (4.135)$$

□

This theorem guarantees the performance of the projective measurement defined below.

Definition 36. For the normal, regular matrix Θ^{est} whose eigenvalues and eigenvectors are given by Eq. (4.116), we define the projective super operator $\tilde{\mathcal{P}}_i^{\Theta^{\text{est}}}$

$$\tilde{\mathcal{P}}_i^{\Theta^{\text{est}}} \rho = \sum_i \tilde{P}_i \rho \tilde{P}_i, \quad (4.136)$$

where

$$\tilde{P}_i = \sum_\alpha \tilde{P}_{i,\alpha}. \quad (4.137)$$

We also define the value of $\tilde{E}_i^{\Theta^{\text{est}}}$ as

$$\tilde{E}_i^{\Theta^{\text{est}}} = i \frac{\text{Log} e^{i\varphi_i}}{t}, \quad (4.138)$$

where Log is the logarithm function for Θ^{est} . A corresponding instrument is defined by

$$\mathcal{I}_i^{\Theta^{\text{est}}} = p(\Theta^{\text{est}}) \mathcal{P}_{i,\Theta^{\text{est}}}, \quad (4.139)$$

where $p(\Theta^{\text{est}})$ is the probability that we obtain a sequence of data D which provides the matrix Θ^{est} as an estimation result.

Definition 37. We define a measurement $\mathcal{M}_{\text{BF}} = \{ \tilde{\mathcal{I}}, \tilde{E}, Q \}$, where

$$Q : = \{ (\Theta^{\text{est}}, i) | \Theta^{\text{est}} \in \mathbb{C}^{2d}, i \in X \}, \quad (4.140)$$

$$\tilde{\mathcal{I}} : = \{ \tilde{\mathcal{I}}_i^{\Theta^{\text{est}}} | (\Theta^{\text{est}}, i) \in Q \}, \quad (4.141)$$

$$E(\Theta^{\text{est}}, i) : = E_i^{\Theta^{\text{est}}}, \quad (4.142)$$

and we call \mathcal{M}_{BF} as the projective measurement implemented via estimator Θ^{est} .

In the following subsection, we abbreviate Θ^{est} dependency of a CP map $\tilde{\mathcal{I}}_i^{\Theta^{\text{est}}}$ and outcome $\tilde{E}_i^{\Theta^{\text{est}}}$ as $\tilde{\mathcal{I}}_i$ or \tilde{E}_i respectively, when dependency is clearly exhibited in the context.

4.4.2 Evaluation of the performance

The effect of the added matrix for diagonalization

Consider we have a normal matrix \tilde{A} on a Hilbert space \mathcal{H} which is different from the diagonalizable matrix A by a matrix V , namely,

$$\tilde{A} = A + V. \quad (4.143)$$

We assume \tilde{A} is still normal. We represent the diagonalization as

$$\tilde{A} = \sum_k \tilde{a}_k \tilde{P}_k, \quad \tilde{P}_k = \sum_\lambda |\tilde{a}_k^\lambda\rangle \langle \tilde{a}_k^\lambda|. \quad (4.144)$$

We also denote a decomposition of A as

$$A = \sum_k a_k P_k, \quad P_k = \sum_\lambda |a_k^\lambda\rangle \langle a_k^\lambda|. \quad (4.145)$$

We decompose the eigenbasis $\{|a_i^\lambda\rangle\}$ of A by the basis $\{|\tilde{a}_i^\lambda\rangle\}$ of \tilde{A} .

$$|a_i^\lambda\rangle = \sum_j \tilde{v}_{ij}^{\lambda\mu} |\tilde{a}_j^\mu\rangle. \quad (4.146)$$

Applying the matrix \tilde{A} to both sides of Eq. (4.146), we have

$$a_i |a_i^\lambda\rangle = \sum_{j,\lambda} \tilde{v}_{ij}^{\lambda\mu} \tilde{a}_j |\tilde{a}_j^\mu\rangle - V |a_i^\lambda\rangle. \quad (4.147)$$

By comparing the coefficients in the eigen basis of A , we obtain

$$\tilde{v}_{ij}^{\lambda\mu} (\tilde{a}_j - a_i) = \tilde{V}_{ij}^{\lambda\mu}, \quad (4.148)$$

where $V_{ij}^{(\lambda\mu)} = \langle \tilde{a}_j^{(\mu)} | V | a_i^\lambda \rangle$. Then the coefficient \tilde{v}_{ij} is determined by

$$\tilde{v}_{ij} = \frac{\tilde{V}_{ij}^{\lambda\mu}}{\tilde{a}_j - a_i}. \quad (4.149)$$

Evaluating fluctuation of measurement value

In the followings, we evaluate the performances of measurements introduced in Sec.4.4. The fluctuation of measurement value for the measurement \mathcal{M}_{BF} is given by

$$R_1(\mathcal{M}_{BF}|H) = \max_{\substack{\{|E_i^\lambda\rangle\} \\ i \in Y, \lambda \in Z_i}} \left\langle \sum_j \langle E_i^\lambda | \tilde{P}_j | E_i^\lambda \rangle (\tilde{E}_j - E_i)^2 \right\rangle_{D, \Theta}^{\text{exp}}. \quad (4.150)$$

We define an orthonormal basis $\{|\tilde{E}_{j;\alpha}^\lambda\rangle\}$ of \tilde{H} determined by the estimator Θ^{est} as follows:

$$|\tilde{E}_{j;\alpha}^0\rangle = \frac{\tilde{P}_{j;\alpha}|E_i^\lambda\rangle}{\sqrt{\langle E_i^\lambda|\tilde{P}_{j;\alpha}|E_i^\lambda\rangle}}, \quad (4.151)$$

where $i \in Y$ and $\lambda \in Z_i$ are chosen as they achieve the maximization in the right-hand side of Eq. (4.150). We define $v_{ij;\alpha}^{\lambda\mu}$ as an inner product of two basis vectors as

$$v_{ij;\alpha}^{\lambda 0} = \langle \tilde{E}_{j;\alpha}^\mu | E_i^\lambda \rangle. \quad (4.152)$$

Because of the definition of $|\tilde{E}_{j;\alpha}^\mu\rangle$, we obtain

$$v_{ij;\alpha}^{\lambda 0} = \frac{\langle E_i^\lambda | \tilde{P}_{j;\alpha} | E_i^\lambda \rangle}{\sqrt{\langle E_i^\lambda | \tilde{P}_{j;\alpha} | E_i^\lambda \rangle}}. \quad (4.153)$$

Then we obtain

$$|v_{ij;\alpha}^{\lambda 0}|^2 = \langle E_i^\lambda | \tilde{P}_{j;\alpha} | E_i^\lambda \rangle. \quad (4.154)$$

Substituting Eq. (4.154) into Eq. (4.150), we have

$$R_1(\mathcal{M}_{BF}|H) = \max_{\substack{\{|E_i^\lambda\rangle\} \\ i \in Y, \lambda \in Z_i}} \left\langle \sum_{j;\alpha} |v_{ij;\alpha}^{\lambda 0}|^2 (\tilde{E}_j - E_i)^2 \right\rangle_{D, \Theta}^{\text{exp}}. \quad (4.155)$$

We assume the estimator Θ^{est} and the unitary U satisfy all the condition imposed in the previous section. We define the following step function according to the $\varphi_{\Theta^{\text{est}}}$ defined in the previous section as

$$s(D) = 0, \quad \left(\varphi_{\Theta^{\text{est}}} \in \left[-\frac{\pi}{2}, \frac{\pi}{2} \right] \right) \quad (4.156)$$

$$= 1, \quad (\text{otherwise}). \quad (4.157)$$

Using $s(D)$, we divide the maximized value in Eq. (4.155) in the definition of R_1 into δ_i, ϵ_i as

$$\delta_i = \left\langle \sum_{j;\alpha} |v_{ij;\alpha}^{\lambda 0}|^2 (\tilde{E}_j - E_i)^2 s(D) \right\rangle_{D, \Theta}^{\text{exp}}, \quad (4.158)$$

$$\epsilon_i = \left\langle \sum_{j;\alpha} |v_{ij;\alpha}^{\lambda 0}|^2 (\tilde{E}_j - E_i)^2 (1 - s(D)) \right\rangle_{D, \Theta}^{\text{exp}}. \quad (4.159)$$

Substituting $V = \Theta^{\text{est}} - \Theta$ into Eq. (4.149), δ_i is transformed to

$$\delta_i = \left\langle \sum_{j;\alpha} \frac{|\tilde{E}_j - E_i|^2}{|c_{j;\alpha} e^{-i\tilde{E}_j t} - c e^{-iE_i t}|^2} |v_{ij;\alpha}^{\lambda 0}|^2 s(D) \right\rangle_{D, \Theta}^{\text{exp}} \quad (4.160)$$

The numerator in the right-hand side of Eq. (4.160) is simplified as

$$\left| c_i^{(0)} e^{-i\tilde{E}_j t} - c e^{-iE_i t} \right|^2 = c^2 + c_{j,\alpha}^2 - 2cc_{j,\alpha} \cos(E_i - \tilde{E}_j)t. \quad (4.161)$$

By differentiating this equation by a parameter c_i , it is shown that the minimum is realized when the parameter $c_{j,\alpha}$ is given by

$$c_{j,\alpha} = c \times \max \left\{ \cos(E_i - \tilde{E}_j)t, 0 \right\}. \quad (4.162)$$

Substituting this result into the equation, we achieve

$$\left| c_{j,\alpha} e^{-i\tilde{E}_j t} - c e^{-iE_i t} \right|^2 \geq c^2 f(x), \quad (4.163)$$

where f is defined as

$$f(x) = \sin^2 x, \quad (\cos x \geq 0), \quad (4.164)$$

$$= 1, \quad (\text{otherwise}). \quad (4.165)$$

Then δ_i is bounded as

$$\delta_i \leq \frac{1}{t^2 c^2} \left\langle \sum_j \frac{(E_i t - \tilde{E}_j t)^2}{f(E_i t - \tilde{E}_j t)} |V_{ij}^{\lambda 0}|^2 s(D) \right\rangle_{D,\Theta}^{\text{exp}}. \quad (4.166)$$

When $s(D) = 1$ is realized, $\varphi_j = -\tilde{E}_j t$ satisfies $\varphi_j \in [-3\pi/2, 3\pi/2]$. According to Eq. (4.115), the value $x = \varphi_j + E_i t$ satisfies $x \in [-5\pi/4 \leq 5\pi/4]$. In this domain, the function $x^2/f(x)$ takes the maximum value $25\pi^2/8$ when $x = \pm 5\pi/4$. Then we achieve the upper bound of δ_i given by

$$\delta_i \leq \frac{25\pi^2}{8t^2 c^2} \left\langle \sum_j |\tilde{V}_{ij}^{\lambda 0}|^2 s(D) \right\rangle_{D,\Theta}^{\text{exp}}. \quad (4.167)$$

Since $s(D) \leq 1$, we further simplify this upper bound as

$$\delta_i \leq \frac{25\pi^2}{8t^2 c^2} \left\langle \sum_j |\tilde{V}_{ij;\alpha}^{\lambda 0}|^2 \right\rangle_{D,\Theta}^{\text{exp}}. \quad (4.168)$$

By using the notation of the trace operation, the value in the parentheses are transformed as

$$\sum_j |\tilde{V}_{ij;\alpha}^{\lambda 0}|^2 = \sum_j |\langle \tilde{E}_j^0 | V | E_i^\lambda \rangle|^2 \quad (4.169)$$

$$= \sum_j \langle \tilde{E}_j^0 | V | E_i^\lambda \rangle \langle E_i^\lambda | V^\dagger | \tilde{E}_j^0 \rangle \quad (4.170)$$

$$\leq \text{Tr} [V | E_i^\lambda \rangle \langle E_i^\lambda | V^\dagger] \quad (4.171)$$

$$= \langle E_i^\lambda | |V|^2 | E_i^\lambda \rangle \quad (4.172)$$

$$= Y_i^\lambda, \quad (4.173)$$

where Y_i is defined as Eq. (4.124).

Using Theorem 7 and $1/\sqrt{2} \leq c \leq 1$ to this inequality, we conclude that

$$\delta_i \leq \frac{25\pi^2}{4t^2M}. \quad (4.174)$$

Next, we evaluate ϵ_i . By definition, E_i and \tilde{E}_j are bounded by

$$|E_it| \leq \pi/4, \quad |\tilde{E}_jt| \leq 2\pi. \quad (4.175)$$

Then we have

$$|E_it - \tilde{E}_jt| \leq \frac{9\pi}{4}. \quad (4.176)$$

Thus ϵ_i is bounded as

$$\epsilon_i \leq \frac{81\pi^2}{16t^2} \langle (1 - s(D)) \rangle_{D,\Theta}^{\text{exp}}. \quad (4.177)$$

Because of the definition of $s(D)$, we can replace the expectation value part of the inequality by $P\{\varphi_\Theta \in [-\pi/2, \pi/2]\}$. Then according to Theorem 8, we obtain

$$\epsilon_i \leq \frac{81d\pi^2}{t^2} \left(\frac{12}{M} + \frac{9}{M^2} \right). \quad (4.178)$$

Since $\max_i(\delta_i + \epsilon_i)$ gives the fluctuation of measurement value and the upper bound of each ϵ_i and δ_i is determined, $R_1(\mathcal{M}_{BF}|H)$ is bounded as

$$R_1(\mathcal{M}_{BF}|H) \leq \frac{\pi^2}{t^2} \left(\frac{25}{4M} + \frac{972d}{M} + \frac{729d}{M^2} \right). \quad (4.179)$$

The above discussions are summarized in the following theorem.

Theorem 10. *Assume that an estimator Θ^{est} for the parameter Θ satisfies the conditions given by Eqs. (4.80),(4.81) and the conditions of normality and regularity. We also assume that the matrix Θ is determined by a Hamiltonian H satisfying Eqs. (4.108),(4.109) and (4.113), and the parameter t satisfies $\Delta_{\max}t < \pi/4$. Then the measurement \mathcal{M}_{BF} according to this estimator satisfies.*

$$R_1(\mathcal{M}_{BF}|H) \leq \frac{\pi^2}{t^2} \left(\frac{25}{4M} + \frac{972d}{M} + \frac{729d}{M^2} \right). \quad (4.180)$$

About non-repeatability R_2 of this tomography based measurement scheme, no obvious bound has been found. However, it is conceivable that no matter how many times we iterate measurements to identify Θ , R_2 is not always concentrated to zero. Consider the case that the system is two dimensional ($d = 2$) and its Hamiltonian is degenerated $H = E_0I$. The projective measurement of energy

for this Hamiltonian has only one measurement instrument id, which means that the measurement operation affecting the system after obtaining an outcome is an identity operation id, (namely, the state does not change). On the other hand, the parameter Θ for this case is given as I . The estimated matrix Θ^{est} is given by

$$\Theta^{\text{est}} = I + V, \quad (4.181)$$

where V is the statistical error from the true parameter Θ . Again we assume that V is a normal matrix. According to Eq. (4.181), it is clear that the eigenbasis of Θ^{est} is equal to the ones of V . Normal matrices are completely represented by parameters describing eigenbasis and eigenvalues. A set of degenerated matrices is described as a set of the parameters whose eigenvalue part has a restriction. Then the set of degenerated matrix is a zero set in this parameter space. According to this fact, we assume that the event of matrix Θ^{est} having degenerated eigenvalues is zero. Then the CPTP map according to the measurement \mathcal{M}_{BF} can be rewritten as

$$\sum_{i=1,2} \sum_{\Theta^{\text{est}}} \mathcal{I}_{i,\Theta^{\text{est}}} = \sum_{\Theta^{\text{est}}} p(\Theta^{\text{est}}) \Lambda_{\Theta^{\text{est}}}, \quad (4.182)$$

where

$$\Lambda_{\Theta^{\text{est}}} = \sum_{i=1,2} \tilde{\mathcal{P}}_{i,\Theta^{\text{est}}}. \quad (4.183)$$

Consider a maximally entangled state ρ_{me} on a two-qubit system $\mathbb{C}^2 \otimes \mathbb{C}^2$. By applying $\Lambda_{\Theta^{\text{est}}}$ to the first qubit of the maximally entangled state, the state after the measurement operation becomes a separable state. We call such an operation as an entanglement breaking operation. A convex sum of separable states is also a separable state by definition. Then a convex sum of a entanglement breaking operation is still entanglement breaking operation. We define a separable state ρ_{sep} as

$$\rho_{\text{sep}} = \langle \Lambda_{\Theta^{\text{est}}} \rho \rangle_{D,\Theta}^{\text{exp}} = \sum_{\Theta^{\text{est}}} p(\Theta^{\text{est}}) \Lambda_{\Theta^{\text{est}}} \rho_{\text{me}}. \quad (4.184)$$

Note that $\langle \Lambda_{\Theta^{\text{est}}} \rho \rangle_{D,\Theta}^{\text{exp}}$ is equivalent to the CPTP map corresponding to the measurement \mathcal{M}_{BF} . For this case, non-repeatability R_2 is calculated as

$$R_2(\mathcal{M}_{BF}|H) = \max_{\rho \in D(\mathbb{C}^2 \times \mathbb{C}^2)} \left\| \langle \Lambda_{\Theta^{\text{est}}} \rho \rangle_{D,\Theta}^{\text{exp}} - \rho \right\|_{tr}.$$

Because of the maximization of the value in the right-hand side, if we substitute the state ρ to ρ_{me} , the value is smaller than the maximized value, namely,

$$R_2(\mathcal{M}_{BF}|H) \geq \left\| \rho_{\text{sep}} - \rho_{\text{me}} \right\|_{tr}. \quad (4.185)$$

The trace norm satisfies the non-negativity condition $\|\rho - \sigma\|_{tr} = 0 \Leftrightarrow \rho = \sigma$. A set of separable states does not include a maximally entangled state nor a sequence which approaches to a maximally entangled state, because entanglement measures are continuous functions and separable states have zero entanglement, on the other hand maximally entangled states have nonzero value. Then there is a constant $c > 0$ which satisfies

$$R_2(\mathcal{M}_{BF}|H) \geq c. \quad (4.186)$$

Then we find that there exists the case where R_2 does not concentrate into zero even if we iterate measurements for infinite times.

Evaluation of the runtime to achieve the required precision

The fluctuation of measurement value is the mean squared error of measurement outcomes from the true value. In the following, we calculate the sufficient runtime to achieve required accuracy ε , namely,

$$R_1(\mathcal{M}_{BF}) \leq \varepsilon. \quad (4.187)$$

The total time to implement the energy measurement via Hamiltonian tomography is divided into the time for the Schrödinger evolution of the system and the time required for our manipulation, (for example, preparation of initial states, executing measurements for process tomography and implementation of the projective measurement of energy). The latter depends on how fast we can execute manipulation, and it is not bounded in principle. Then the total calling time of the Schrödinger evolution is the ideal bound of the total time [2, 5, 12].

To implement \mathcal{M}_{BF} , according to Sec. 4.3 we must prepare $4d - 3$ different initial states and perform d^2 different measurements on each state after applying the Hamiltonian dynamics with duration time t . If we iterate measurement M times for each combination, the time is determined by

$$T_{BF} = M \times (4d - 3) \times d^2 \times t. \quad (4.188)$$

Due to Eq. (4.180), M must satisfy $M > O(d/(t^2\varepsilon))$ to achieve Eq. (4.187). Then

$$T_{BF} > O\left(\frac{d^4}{t\varepsilon}\right), \quad (4.189)$$

is the sufficient runtime for achieving the inequality. When a bound of the maximum eigenvalue difference in eigenvalues Δ_{max} is known, due to the assumption

$\pi/4 \geq \Delta_{\max}t$, we can minimize the upper bound of the total time. If we take $t = \Delta_{\max}/\pi$, then the ideal bound of the runtime is given by

$$T_{BF} > O\left(\frac{d^4 \Delta_{\max}}{\varepsilon}\right). \quad (4.190)$$

Chapter 5

Phase estimation based method: algorithm and evaluation

5.1 Introduction

In this chapter, we present a method to implement projective measurement of energy on any finite dimensional system whose self-Hamiltonian is unknown. This method achieves the ideal projective measurement of energy in the limit of infinite time resource, while its run time for a given accuracy is independent of the system dimension. We introduce a randomization technique to show that a quantum algorithm known as a quantum phase estimation algorithm [18] can be applied to a system evolving under an unknown Hamiltonian whose bound on the maximum difference in the energy eigenvalues is known. More specifically, by using our technique we show that a unitary operation conditioned on a quantum input (i.e., a controlled-unitary operation) can be implemented for an unknown unitary operation provided as a physical system evolving according to an unknown Hamiltonian. In contrast, previously known implementations of the conditional operations require that the unitary operation to be controlled is known, at least partially [22, 23].

In Sec. 5.2, we introduce the phase estimation algorithm which asymptotically implements projective measurement of energy by using the controlled Hamiltonian dynamics of the target system as resource. In Sec. 5.3, we introduce our new algorithm *universal controllization* which utilizes Hamiltonian evolution of closed quantum dynamics for implementing the controlled version of Hamiltonian evolution. In Sec. 5.4 we apply the universal controllization to the phase estimation algorithm, In Sec. 5.5 we analyze the performance of the implemented projective measurement of energy. Finally, we evaluate the necessary running time to guarantee small fluctuation outcome for the energy measurement in Sec. 5.6.

5.2 Phase estimation algorithm

The phase estimation algorithm is a quantum algorithm to estimate the phase factor $0 \leq \theta_i < 2\pi$ of the eigenvalue $e^{i\theta_i}$ of a finite dimensional unitary operation U when an eigenstate $|\theta_i^\lambda\rangle$ is given. A spectral decomposition of U is given by

$$U(t) = \sum_{k \in Y} e^{i\theta_k} P_k, \quad P_k = \sum_{\lambda \in Z_k} |\theta_k^\lambda\rangle\langle\theta_k^\lambda|. \quad (5.1)$$

The algorithm is presented by a quantum circuit shown in Fig. 5.1. As shown in the figure, this algorithm uses controlled-unitary operations of $U, U^2, U^4, \dots, U^{2^N}$ where N denotes the number of control qubits. A controlled-unitary operation C_U of a unitary operation U is defined by

$$C_U := |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes U \quad (5.2)$$

on $\mathcal{H}_c \otimes \mathcal{H}_t$ where the Hilbert spaces of the control system and the target system are represented by $\mathcal{H}_c = \mathbb{C}^2$ and $\mathcal{H}_t = \mathbb{C}^d$ ($d < \infty$), respectively.

The final measurement of N control qubits in the computational base provides a sequence of outcomes $\{n_1, \dots, n_N\}$ where $n_k \in \{0, 1\}$ corresponds to the measurement outcome of the k -th control qubit. Then the estimated phase is given by $2\pi f_N$ where $f_N := 0.n_1 \dots n_N$ is the binary representation of a decimal number defined by $0.n_1 \dots n_N := \sum_{k=1}^N 2^{-k} n_k$. When an input state of the target system is $|\theta_i^\lambda\rangle$, the probability of obtaining $2\pi f_N$ is

$$P_N(2\pi f_N | \theta_i^\lambda) = \left(\frac{\sin [2^N (\theta_i - 2\pi f_N) / 2]}{2^N \sin [(\theta_i - 2\pi f_N) / 2]} \right)^2. \quad (5.3)$$

We show this result in Sec. 5.4. The output state of the target system remains in $|\theta_i\rangle$. The probability distribution of the estimation error $y := \theta_i - 2\pi f_N$ is given by

$$p_N(y) := P_N(\theta_i - y | \theta_i^\lambda) = \left(\frac{\sin [2^N y / 2]}{2^N \sin [y / 2]} \right)^2. \quad (5.4)$$

This means that $p_N(y)$ for $y \neq 0$ decreases exponentially in N . The function $p_N(y)$ can be regarded as a probability distribution of a discrete random variable $y_n^\Delta = 2\pi(n + \Delta) / 2^N$ with $-2^{N-1} \leq n < 2^{N-1}$ satisfying

$$\sum_{n=-2^{N-1}}^{2^{N-1}-1} p_N(y_n^\Delta) = 1 \quad (5.5)$$

where $-1/2 \leq \Delta < 1/2$. We show that this discrete probability distribution converges to a delta function on the section $[-\pi, \pi]$ at $N \rightarrow \infty$.

To transform a discrete random variable to a continuous one, we construct a probability measure μ corresponding to the probability distribution p_N^Δ at the limit $N \rightarrow \infty$. The measure is naturally defined by

$$\mu(A) = \lim_{N \rightarrow \infty} \sum_{y_n^\Delta \in A} p_N(y_n^\Delta), \quad (5.6)$$

where A is a subset of $[-\pi, \pi]$. If $A = [a, b]$ for $a, b > 0$, we can bound $\mu(A)$ as

$$\mu(A) \leq \lim_{N \rightarrow \infty} N_A \left(\frac{1}{2^N \sin a} \right)^2. \quad (5.7)$$

Since $N_A \leq (b - a)(2^N + 1)$,

$$0 \leq \mu(A) \leq \frac{b - a}{\sin^2 a} \lim_{N \rightarrow \infty} \frac{2^N + 1}{2^{2N}} = 0. \quad (5.8)$$

This implies $\mu(A) = 0$. If $A = [a, b]$ for $a, b < 0$, we can similarly obtain $\mu(A) = 0$. Thus $\mu(A) = 1$ should be satisfied in the case of $a < 0 < b$ due to Eq. (5.5).

We define a set of functions \mathcal{F} of which elements are measurable and continuous at $x = 0$. Integral of $f \in \{\mathcal{F}\}$ over the section $[-\pi, \pi]$ by the probability measure μ is represented by

$$\int_{-\pi}^{\pi} \mu(dx) f(x) = \lim_{n \rightarrow \infty} \sum_{k=-\infty}^{\infty} \frac{k}{n} \mu(A_k^n) \quad (5.9)$$

where $A_k^n = f^{-1}([k/n, (k+1)/n])$. This definition of integral is well defined due to the condition of f to be measurable.

There is an integer i such that $\{f(0)\} \in A_i^\circ$ (or $\{f(0)\} = \bar{A}_i \cap \bar{A}_{i+1}$), where A° denotes the interior of the set A . (\bar{A} means the closure of A .) Due to the continuity, A_i (or $A_i \cup A_{i+1}$) includes a section $[a, b]$ of $a < 0 < b$. Then $\mu(A_i) = 1$ (or $\mu(A_i) + \mu(A_{i+1}) = 1$) should be satisfied. Thus the integral satisfies

$$\int_{-\pi}^{\pi} f(x) \mu(dx) = f(0). \quad (5.10)$$

Formally, we can represent this probability measure as a probability distribution $p(x)$ of a continuous random variable x ,

$$\int_{-\pi}^{\pi} f(x) \mu(dx) = \int_{-\pi}^{\pi} f(x) p(x) dx = f(0). \quad (5.11)$$

Therefore the function p can be regarded as a delta function for the set of functions \mathcal{F} . The set of function \mathcal{F} includes smooth functions that are known as descriptions of physically natural values.

We note that the measure μ is not a measure called the ‘‘Dirac measure’’. The set $A = \{2\pi\Delta/2^N | N \geq 1\}$ has non-zero value under the μ measure, but it gives zero under the Dirac measure.

If we apply the phase estimation algorithm to an arbitrarily superposed input state $|\phi\rangle = \sum_{i,\lambda} \alpha_i^\lambda |\theta_i^\lambda\rangle$ where $\sum_{i,\lambda} |\alpha_i^\lambda|^2 = 1$, the probability distribution of obtaining the outcomes $\{n_1, \dots, n_N\}$ represented in terms of $f_N = 0.n_1 \dots n_N$ is given by

$$P_N(2\pi f_N | \phi) = \sum_{i,\lambda} |\alpha_i^\lambda|^2 P_N(2\pi f_N | \theta_i^\lambda). \quad (5.12)$$

The corresponding output state of the target system is

$$|\phi'_{f_N}\rangle = \frac{\sum_{i,\lambda} \alpha_i^\lambda (P_N(2\pi f_N | \theta_i^\lambda))^{1/2}}{\sqrt{P_N(2\pi f_N | \phi)}} e^{iG(\theta_i, f_N)} |\theta_i^\lambda\rangle, \quad (5.13)$$

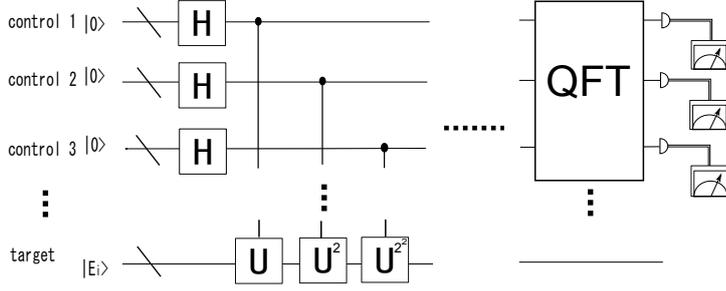


Figure 5.1: The phase estimation algorithm. The box QFT denotes the quantum Fourier transformation. The final measurement is performed in the computational basis.

where $G(\theta_i, f_N) = (2^N - 1)(\theta_i - 2\pi f_N)$. Since $2\pi f_N \rightarrow \theta_i$ is guaranteed for $N \rightarrow \infty$, the output state converges to $P_k|\phi\rangle / \|P_k|\phi\rangle\|$ when the outcome is f_N . Thus the phase estimation algorithm implements a projective measurement in the eigenbasis of U for $N \rightarrow \infty$.

If U is given by a Hamiltonian evolution operator $U(t) = e^{-iHt}$ of a Hamiltonian H , the phase estimation algorithm asymptotically implements a projective measurement of energy on \mathcal{H}_t that gives an outcome representing an energy eigenvalue E_i of H up to periodicity of the phase on \mathcal{H}_t and also gives an instrument $\{\mathcal{P}_i^H\}$ to an eigenstate corresponding to the outcome E_i . This property of the phase estimation algorithm is also used in thermalization algorithms [20, 21].

5.3 Controlling of the quantum dynamics

If we can perform the controlled unitary $C_{U(t)}$, we can implement the projective measurement of energy via the phase estimation algorithm. Unfortunately, with a finite time resource, $C_{U(t)}$ for $U(t) = \exp(-iHt)$ cannot be perfectly implemented when H is unknown. (See Ref. [24], for instance.) We address this issue by implementing an approximated version of $C_{U(t)}$.

Let us denote the Hilbert spaces of the control and the target system by \mathcal{H}_c and \mathcal{H}_t , respectively. First, we add an ancilla system, with Hilbert space $\mathcal{H}_a = \mathbb{C}^d$, and initially prepare it in the completely mixed state I/d . We introduce the *pseudo controlled unitary operation* $W_{U(t/m)}$ of $C_{U(t/m)}$, which is a unitary operation on $\mathcal{H}_c \otimes \mathcal{H}_a \otimes \mathcal{H}_t$, defined by

$$W_{U(t/m)} = \tilde{F}(I \otimes I \otimes U(t/m))\tilde{F}, \quad (5.14)$$

where

$$\tilde{F} = |0\rangle\langle 0| \otimes I \otimes I + |1\rangle\langle 1| \otimes SWAP \quad (5.15)$$

and the unitary operation $SWAP$ on $\mathcal{H}_a \otimes \mathcal{H}_t$ is defined as

$$SWAP|\psi\rangle|\phi\rangle = |\phi\rangle|\psi\rangle, \quad |\psi\rangle|\phi\rangle \in \mathcal{H}_t \otimes \mathcal{H}_c. \quad (5.16)$$

For an input density operator

$$\rho := \sum_{j,k} |j\rangle\langle k| \otimes \frac{I}{d} \otimes \rho_{j,k} \quad (5.17)$$

on $\mathcal{H}_c \otimes \mathcal{H}_a \otimes \mathcal{H}_t$, we see that

$$W_{U(t/m)}\rho W_{U(t/m)}^\dagger = \sum_{j,k} |j\rangle\langle k| \otimes \frac{1}{d} U\left(\frac{(j-k)t}{m}\right) \otimes U\left(\frac{jt}{m}\right) \rho_{j,k} U^\dagger\left(\frac{kt}{m}\right),$$

where $j, k = 0, 1$. The operation $W_{U(t/m)}$ generally entangles the ancilla and the rest of the system.

The entanglement is broken by the use of the following randomization process. We perform m iterations of unitary operation $V_{U(t/m)}^{(r)} = (I \otimes \sigma_r \otimes I) W_{U(t/m)} (I \otimes \sigma_r^\dagger \otimes I)$ on $\mathcal{H}_c \otimes \mathcal{H}_a \otimes \mathcal{H}_t$, where σ_r is uniformly and randomly chosen for each iteration from a set of D operations $\{\sigma_r\}$ such that

$$\frac{1}{D} \sum_r \sigma_r U \sigma_r^\dagger = \text{Tr} U \cdot I, \quad (5.18)$$

for all unitary operators U on \mathcal{H}_t . If the system is composed by a q -qubits, we can use the set of general Pauli matrices $\{\mathcal{X}_i^{(j)}\}$ in Eq. (4.55) as an example. We denote the CPTP map of the randomized $V_{U(t/m)}^{(r)}$ by

$$\mathcal{V}_{U(t/m)}(\rho) := \frac{1}{D} \sum_r V_{U(t/m)}^{(r)} \rho (V_{U(t/m)}^{(r)})^\dagger$$

and define the reduced CPTP map $\Gamma_{U(t/m)}$ of $\mathcal{V}_{U(t/m)}$ on $\mathcal{H}_c \otimes \mathcal{H}_t$ for the reduced state $\rho_{ct} := \text{Tr}_{\mathcal{H}_a} \rho$ by

$$\Gamma_{U(t/m)}(\rho_{ct}) := \text{Tr}_{\mathcal{H}_a} [\mathcal{V}_{U(t/m)}(\rho_{ct} \otimes I/d)]. \quad (5.19)$$

The randomization process transforms all components on \mathcal{H}_a to states proportional to the completely mixed state, hence $\mathcal{V}_{U(t/m)}(\rho_{ct} \otimes I/d) = \Gamma_{U(t/m)}(\rho_{ct}) \otimes I/d$. Random operations are used in a similar spirit when decoupling a system from an interacting environment as the dynamical decoupling [25], but in this case

the random operations are applied on the system. See Fig. 5.2(b) for a quantum circuit representation of the algorithm.

Let us analyze the accuracy of the approximation. For m iterations of the maps $\Gamma_{U(t/m)}$ and $\mathcal{V}_{U(t/m)}$ (denoted by $\Gamma_{U(t/m)}^m$ and $\mathcal{V}_{U(t/m)}^m$, respectively), we have

$$\Gamma_{U(t/m)}^m(\rho_{ct}) = \text{Tr}[\mathcal{V}_{U(t/m)}^m(\rho_{ct} \otimes I/d)]. \quad (5.20)$$

We define a controlled unitary ‘‘up to phases’’ by

$$C_U^{(g_U)} := [|0\rangle\langle 0| \otimes I + e^{ig_U}|1\rangle\langle 1| \otimes U], \quad (5.21)$$

where g_U is a real function of U . Let $C_U^{(g_U)}$ be the CPTP map representing unitary operation $C_U^{(g_U)}$.

We evaluate the difference between the two CPTP maps $C_{U(t)}^{(m\varphi_{U(t/m)})}$ and $\Gamma_{U(t/m)}^m$ in terms of the diamond norm. Both maps act on the Hilbert space $\mathcal{H}_c \otimes \mathcal{H}_t = \mathbb{C}^2 \otimes \mathbb{C}^d$. Thus we search rank-1 projectors on $(\mathcal{H}_c \otimes \mathcal{H}_t)^{\otimes 2}$ to calculate the diamond norm. (According to Lemma. 1.) Any vector $|\Psi\rangle$ in $(\mathcal{H}_c \otimes \mathcal{H}_t)^{\otimes 2}$ can be represented by $|\Psi\rangle = \alpha|0\rangle|\psi\rangle + \beta|1\rangle|\phi\rangle$ where $\{|0\rangle, |1\rangle\}$ is the computational basis of the first control qubit system \mathcal{H}_c , by taking appropriate states $|\psi\rangle, |\phi\rangle \in \mathcal{H}_c \otimes \mathcal{H}_t$ and α, β satisfying $|\alpha|^2 + |\beta|^2 = 1$. Any rank-1 operator on $(\mathcal{H}_c \otimes \mathcal{H}_t)^{\otimes 2}$ can be written by $|\Psi\rangle\langle\Psi|$.

As a partitioned matrix, the projector is represented by

$$|\Psi\rangle\langle\Psi| = \begin{pmatrix} |\alpha|^2 |\psi\rangle\langle\psi| & \alpha\beta^* |\psi\rangle\langle\phi| \\ \alpha^*\beta |\phi\rangle\langle\psi| & |\beta|^2 |\phi\rangle\langle\phi| \end{pmatrix}. \quad (5.22)$$

The left upper partition corresponds to the $|0\rangle\langle 0|$ element of the first system represented by $\mathcal{H}_c = \mathbb{C}^2$. The right upper partition is the $|0\rangle\langle 1|$ element, and so as the others. The projector $|\Psi\rangle\langle\Psi|$ is transformed by the maps $C_{U(t)}^{(m\varphi_{U(t/m)})}$ and $\Gamma_{U(t/m)}^m$ on $\mathcal{H}_c \otimes \mathcal{H}_t$ as

$$\left(C_{U(t)}^{(m\varphi_{U(t/m)})} \otimes \mathcal{I}_{\mathcal{H}_c \otimes \mathcal{H}_t} \right) [|\Psi\rangle\langle\Psi|] = \begin{pmatrix} |\alpha|^2 |\psi\rangle\langle\psi| & \alpha\beta^* e^{-im\varphi_{U(t/m)}} |\psi\rangle\langle\phi| U(t)^\dagger \\ \alpha^*\beta e^{im\varphi_{U(t/m)}} U(t)|\phi\rangle\langle\psi| & |\beta|^2 U(t)|\phi\rangle\langle\phi| U(t)^\dagger \end{pmatrix} \quad (5.23)$$

and

$$\left(\Gamma_{U(t/m)}^m \otimes \text{id}_{\mathcal{H}_c \otimes \mathcal{H}_t} \right) [|\Psi\rangle\langle\Psi|] = \begin{pmatrix} |\alpha|^2 |\psi\rangle\langle\psi| & \text{Tr} \left[U\left(\frac{t}{m}\right)^m \alpha\beta^* |\psi\rangle\langle\phi| U(t)^\dagger \right] \\ \text{Tr} \left[U^\dagger\left(\frac{t}{m}\right)^m \alpha^*\beta U(t)|\phi\rangle\langle\psi| \right] & |\beta|^2 U(t)|\phi\rangle\langle\phi| U(t)^\dagger \end{pmatrix}. \quad (5.24)$$

Here, $U(t)$ acts on the first \mathcal{H}_t . Note that

$$\text{Tr} \left[U\left(\frac{t}{m}\right)^m \right] = (a_{U(t/m)})^m e^{-im\varphi_{U(t/m)}} \quad (5.25)$$

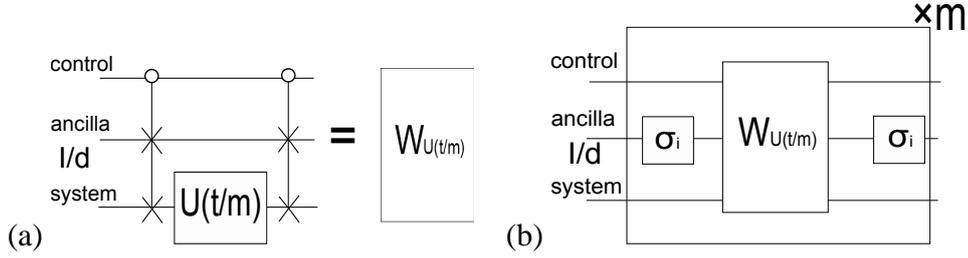


Figure 5.2: (a) Quantum circuit representation of the gate $W_{U(t/m)}$. (b) Quantum circuit representation of the algorithm implementing the approximated $C_{U(t)}$. The two operations σ_i in a sequence are identical, but are chosen randomly for each iteration.

where we shall assume $e^{im\varphi(t/m)} = 1$ for simplicity. (The final consequence is the same for general cases.) Then the norm we are interested in is calculated to be

$$\begin{aligned}
\left\| C_{U(t)}^{(m\varphi_{U(t/m)})} - \Gamma_{U(t/m)}^m \right\|_{\diamond} &= \max_{\substack{|\psi\rangle, |\phi\rangle \\ \alpha, \beta}} (1 - (a_{U(t/m)})^m) \left\| \begin{pmatrix} 0 & \alpha\beta^* |\psi\rangle\langle\phi| U^\dagger \\ \alpha^* \beta U |\phi\rangle\langle\psi| & 0 \end{pmatrix} \right\|_{tr} \\
&= (1 - (a_{U(t/m)})^m) \max_{\substack{|\psi\rangle, |\phi\rangle \\ \alpha, \beta}} |\alpha\beta| \left\| \begin{pmatrix} |\psi\rangle\langle\psi| & 0 \\ 0 & U |\phi\rangle\langle\phi| U^\dagger \end{pmatrix} \right\|_{tr} \\
&= 2(1 - (a_{U(t/m)})^m) \max_{\alpha, \beta} |\alpha\beta| \\
&= 1 - (a_{U(t/m)})^m.
\end{aligned}$$

We refer to $(a_{U(t/m)})^m$ as the *coherence factor* and represents the quality of the approximation. We also define a phase factor $\varphi_{U(t/m)} \in [E_{\max}t/m, E_{\min}t/m]$ so that

$$e^{-i\varphi_{U(t/m)}} = \frac{\text{Tr}[U(t/m)]}{|\text{Tr}[U(t/m)]|}. \quad (5.26)$$

Let $\Delta_{\max} := E_{\max} - E_{\min}$ be the maximum difference between the maximum energy eigenvalues and the minimum energy eigenvalues, then $\varphi_{U(t/m)}$ is determined uniquely, whenever $\Delta_{\max}t \leq \pi/2$. The following value is also uniquely determined

$$E_i t - m\varphi_{U(t/m)} \in [-\pi, \pi]. \quad (5.27)$$

For $\Delta_{\max}t < \pi/2$, the quantity $a_{U(t/m)}$ satisfies

$$a_{U(t/m)} \geq \sqrt{\cos(\Delta_{\max}t/m)} \geq 1 - \frac{(\Delta_{\max})^2 t^2}{4m^2}. \quad (5.28)$$

The total relative phase factor $e^{-im\varphi(t/m)}$, which is obtained by m times the relative phase factor for each iteration $e^{-i\varphi(t/m)}$ converges to $\langle E \rangle t$ at $m \rightarrow \infty$, where $\langle E \rangle$ is the average of the all energy eigenvalues of H , namely,

$$\langle E \rangle = \sum_i d_i \frac{E_i}{d}, \quad d_i = \text{Tr}[P_i]. \quad (5.29)$$

(We have omitted the degeneracy parameter of the energy eigenbasis for simplicity). This statement is shown by the following way. Since $a_{U(t/m)} = 1 + O(1/m^2)$, the coherence factor can be sorted by the order of m as

$$e^{-mi\varphi(t/m)} = \left(1 - i \frac{\text{Tr}[H]t}{dm} + O\left(\frac{1}{m^2}\right) \right)^m. \quad (5.30)$$

Since $\text{Tr}[H]/d = \langle E \rangle$, we can conclude that

$$\begin{aligned} e^{-mi\varphi(t/m)} &= \left(1 - i \frac{\text{Tr}[H]t}{dm} \right)^m + O\left(\frac{1}{m}\right) \\ &= e^{-i\langle E \rangle t} + O\left(\frac{1}{m}\right). \end{aligned}$$

5.4 Applying universal control to phase estimation

In this section, we show the derivation of the probability $Q_N(2\pi f_N|\theta_i, U(t/m))$ of the phase estimation algorithm using universal controllization. $P_N(2\pi f_N|\theta_i)$ is given as the special case of $Q_N(2\pi f_N|\theta_i, U(t/m))$. A spectral decomposition of $U(t) = \exp(-iHt)$ is given by

$$U(t) = \sum_{k \in Y} e^{-iE_k t} P_k, \quad P_k = \sum_{\lambda \in Z_k} |E_k^\lambda\rangle \langle E_k^\lambda|. \quad (5.31)$$

Define $\theta_k \in [0, 2\pi)$ so that

$$\theta_k = -E_k t + 2\pi\nu, \quad \nu \in \mathbb{Z}. \quad (5.32)$$

Let us replace each $C_{U^{2^k}(t)}$ with the approximated map $\Gamma_{U(t/m)}^{m2^k}$ in the phase estimation algorithm.

To estimate the phase in the N -digits precession $2\pi f_N$, we use a system consisting of a target system \mathcal{H}_t and a control system consisting of N -qubit systems $\mathcal{H}_c^{\otimes N}$. The controlled-unitary operation of U^{2^k} denoted by $C_{U^{2^k}}$ is applied on the k -th qubit of the control system.

The initial state of the control and target system is given by

$$|0 \dots 0\rangle \langle 0 \dots 0| \otimes |\theta_i\rangle \langle \theta_i|, \quad (5.33)$$

on $\mathcal{H}_c^{\otimes N} \otimes \mathcal{H}_t$ where $|0 \dots 0\rangle = |0\rangle \otimes \dots \otimes |0\rangle \in \mathcal{H}_c^{\otimes N}$ is a state in the computational basis corresponding to a binary number $0 \dots 0$.

At the first step of the algorithm, the Hadamard gate is applied to each control qubit system. The Hadamard H_{gate} gate is a unitary operation for a single qubit system which is defined as

$$H_{gate} = \frac{1}{2} (|0\rangle\langle 0| + |1\rangle\langle 0| + |0\rangle\langle 1| - |1\rangle\langle 1|). \quad (5.34)$$

The state after this operation is written by

$$\frac{1}{2^N} \sum_{\substack{a_1, a_2, \dots, a_N \\ b_1, b_2, \dots, b_N}} |a_1 a_2 \dots a_N\rangle \langle b_1 b_2 \dots b_N| \otimes |\theta_i\rangle \langle \theta_i| \quad (5.35)$$

where $a_k, b_k \in \{0, 1\}$.

At the second step, the universal controllization map of U^{2^k} , $\Gamma_{U^{2^k}(t/m)}^m$, is applied on the k -th control qubit and the target system for all $1 \leq k \leq N$. After this step, the state is transformed to

$$\begin{aligned} & \frac{1}{2^N} \sum_{\substack{a_1, a_2, \dots, a_N \\ b_1, b_2, \dots, b_N}} \prod_{k=1}^N (a_{U(t/m)})^{m2^k|a_k - b_k|} \exp(i2^{k-1}(a_k - b_k)(\theta_i - m\varphi_{U(t/m)})) \\ & \times |a_1, a_2 \dots a_N\rangle \langle b_1 b_2 \dots b_N| \otimes |\theta_i\rangle \langle \theta_i|. \quad (5.36) \end{aligned}$$

At the last step, the inverse quantum Fourier transformation[36] is applied and then the control qubits are measured in the computational basis. This is equivalent to perform a projective measurement in the Fourier basis $\{|f_N\rangle \langle f_N|\}$ on $\mathcal{H}_c^{\otimes N}$ where

$$|f_N\rangle := \frac{1}{\sqrt{2^N}} \sum_{c_1, c_2, \dots, c_N} e^{-i2^k \pi f_N c_k} |c_1 c_2 \dots c_N\rangle. \quad (5.37)$$

The probability of obtaining f_N by the measurement $\{|f_N\rangle \langle f_N|\}$ on a density operator ρ is given by $\langle f_N | \rho | f_N \rangle$. Thus, the probability distribution $Q_N(2\pi f_N | \theta_i, U(t/m))$

is

$$Q_N(2\pi f_N|\theta_i, U(t/m)) =$$

$$\begin{aligned} & \frac{1}{2^N} \sum_{\substack{a_1, a_2, \dots, a_N \\ b_1, b_2, \dots, b_N}} \prod_{k=1}^N (a_{U(t/m)})^{m2^k|a_k - b_k|} \\ & \quad \times \exp\left(i2^{k-1}(a_k - b_k)(\theta_i + m\varphi_{U(t/m)} - 2\pi f_N)\right) \\ & = \frac{1}{2^N} \prod_{k=1}^N \frac{1}{2} \sum_{a_k, b_k} (a_{U(t/m)})^{m2^k|a_k - b_k|} \\ & \quad \times \exp\left(i2^{k-1}(a_k - b_k)(\theta_i + m\varphi_{U(t/m)} - 2\pi f_N)\right) \\ & = \frac{1}{2^N} \prod_{k=1}^N \left(1 + (a_{U(t/m)})^{m2^k}\right) \\ & \quad \times \cos 2^{k-1}(\theta_i + m\varphi_{U(t/m)} - 2\pi f_N). \end{aligned}$$

The probability distribution $P_N(2\pi f_N|\theta_i)$ corresponds to a special case of $Q_N(2\pi f_N|\theta_i, U(t/m))$ where $a_{U(t/m)} = 1$ and $\varphi_{U(t/m)} = 0$, namely,

$$P_N(2\pi f_N|\theta_i) = \frac{1}{2^N} \prod_{k=1}^N \left(1 + \cos\left(2^{k-1}(\theta_i - 2\pi f_N)\right)\right). \quad (5.38)$$

This probability distribution is simplified in the form given by Eq. (5.3),

$$P_N(2\pi f_N|\theta_i) = \left(\frac{\sin 2^N(\theta_i - 2\pi f_N)/2}{2^N \sin(\theta_i - f_N)/2}\right)^2. \quad (5.39)$$

by using a formula

$$\frac{1}{2^N} \prod_{k=1}^N (1 + \cos 2^{k-1}x) = \left(\frac{\sin 2^N x/2}{2^N \sin x/2}\right)^2, \quad (5.40)$$

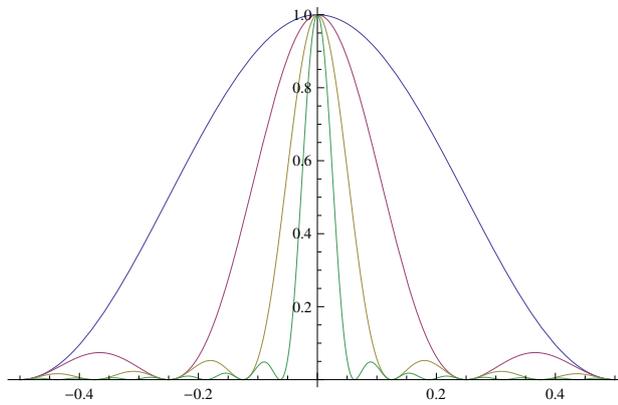
which is obtained by repeatedly using

$$1 + \cos x = \frac{1}{2} \left(\frac{\sin x}{\sin \frac{x}{2}}\right)^2. \quad (5.41)$$

Eq. (5.41) is obtained by combining the following two formulae

$$1 + \cos x = 2 \cos^2 \frac{x}{2}, \quad \cos x = \frac{\sin 2x}{2 \sin x}. \quad (5.42)$$

In Fig. 5.3, we show the probability distributions for several different coherent factors. We can see that the sharpness of each distribution saturates at some number of the control qubits N when $(a_{U(t/m)})^m$ is not equal to 1.



(a) the ideal case

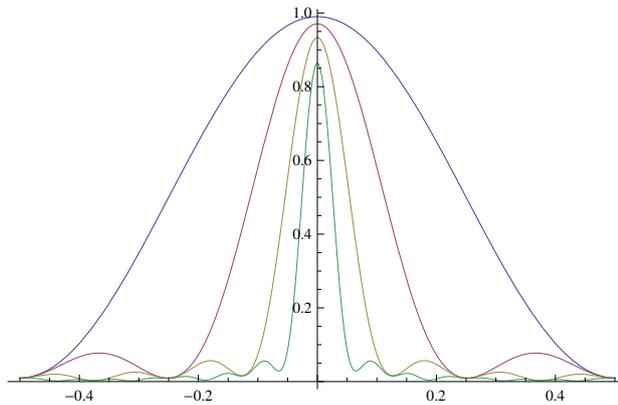
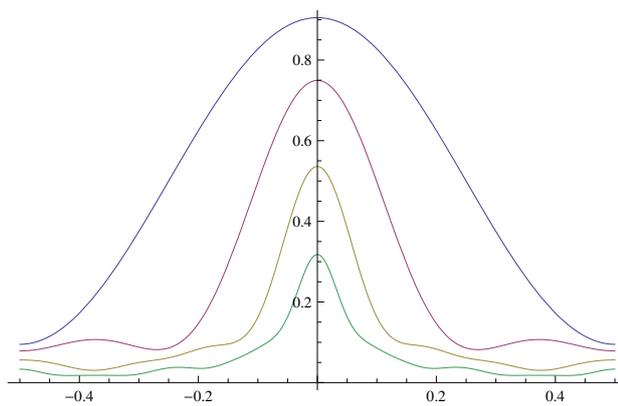
(b) $a_{U(t)} = 0.99$ (c) $a_{U(t)} = 0.9$

Figure 5.3: Probability distributions of phase estimation $Q_N(2\pi f_N|\theta_i)$ for $\theta_i = 0$ and $\varphi_{U(\frac{t}{m})} = 0$ for (a) $a_{U(t/m)} = 1$ (b) $a_{U(t/m)} = 0.99$ (c) $a_{U(t/m)} = 0.9$. The blue lines are for $N = 1$, the red lines are for $N = 2$, the yellow lines are for $N = 3$ and the green lines are for $N = 4$.

The probability distribution of f_N given an eigenvector $|\theta_k\rangle$ of θ_k is

$$Q_N(2\pi f_N | \theta_i, U(t/m)) = \prod_{k=1}^N \frac{1}{2} [1 + (a_{U(t/m)})^{m2^k} \cos 2^{k-1}(\theta_k + m\varphi_{U(t/m)} - 2\pi f_N)]. \quad (5.43)$$

We observe that if the coherence factor satisfies

$$1 - (a_{U(t/m)})^{m2^N} \leq \frac{\delta}{N} \quad (5.44)$$

for a fixed $\delta \in [0, 1/2]$ and $\forall N \in \mathbb{N}$, the probability distribution Q_N satisfies

$$\left| Q_N(2\pi f_N | \theta_k, U(t/m)) - P_N(2\pi f_N | \theta_k + m\varphi_{U(t/m)}) \right| \leq e^\delta - 1 \leq 2\delta. \quad (5.45)$$

To satisfy Eq.(5.44), it suffices to have

$$m \geq \frac{(\Delta_{\max})^2 t^2 N 2^N}{4\delta}. \quad (5.46)$$

5.5 The performance of the measurement

According to Sec. 5.2 and Sec. 5.4, the exact projective measurement of energy for unknown H is implementable with infinite time resource. On the other hand, the projective measurement of energy of unknown H can only be approximated under finite time resource. An approximated projective measurement of energy will show deviations from the ideal behaviors. The accuracy of implementation can be measured by quantifying these deviations by the quantities R_1 and R_2 we defined in Chapter 3. Assume that we know a bound of the maximum energy difference Δ_{\max} in the following process.

Using phase estimation algorithm via universal controllization, we estimate the energy eigenvalues for a given f_N according to

$$E(f_N) = \begin{cases} -2\pi f_N/t & \text{for } f_N \in [0, 1/2) \\ -(2\pi f_N - 2\pi)/t & \text{for } f_N \in [1/2, 1) \end{cases}, \quad (5.47)$$

where we take sufficiently small t satisfying $\Delta_{\max} t \leq \pi/2$. We define the corresponding measurement instruments of the phase estimation algorithm as $\mathcal{I}_{PEA} = \{\mathcal{I}_{f_N}\}$ and measurement as $\mathcal{M}_{PEA} = \{\mathcal{I}_{PEA}, E(f_N), \{f_N\}\}$.

Let \mathcal{M}_{PEA} denote the measurement implemented by our method based on the phase estimation algorithm and define $\tilde{H} = H - (m\varphi_{U(t/m)}/t)I$. A spectral decomposition of \tilde{H} is given by

$$\tilde{H} = \sum_{k \in Y} \tilde{E}_k P_k. \quad (5.48)$$

Notice that $\tilde{E}_k = E_k - m\varphi_{U(t/m)}/t$. The distance between \mathcal{M}_{PEA} and projective measurement of energy of \tilde{H} in terms of R_1 is

$$R_1(\mathcal{M}_{PEA}|\tilde{H}) = \max_{\lambda,k} \sum_{f_N} \text{Tr} \left[\mathcal{I}_{f_N}(|E_k^\lambda\rangle\langle E_k^\lambda|) \right] (\tilde{E}_k - E(f_N))^2. \quad (5.49)$$

Note that

$$\text{Tr} \left[\mathcal{I}_{f_N}(|E_k^\lambda\rangle\langle E_k^\lambda|) \right] = \mathcal{Q}_N(2\pi f_N|\theta_k, U(t/m)). \quad (5.50)$$

In addition,

$$\max_x f(x) \leq \max_x g(x) + \max_y |f(y) - g(y)|. \quad (5.51)$$

If $\Delta_{\max}t < \pi/2$, we have $\tilde{E}_k \in (-\pi/t, \pi/t)$, thus $|\tilde{E}_k - E(f_N)| \leq 2\pi/t$. Therefore, when Eq. (5.45) holds,

$$R_1(\mathcal{M}_{PEA}|\tilde{H}) \leq R_1(\mathcal{M}_{C_{U(t)}}|\tilde{H}) + \frac{2^N(2\delta)4\pi^2}{t^2}, \quad (5.52)$$

where $\mathcal{M}_{C_{U(t)}}$ denotes the measurement implemented by using the ideal controlled unitary operation $C_{U(t)}$.

We set $m\varphi_{U(t/m)} = 0$ for brevity. If an ideal controlled-unitary operation $C_{U(t)}$ is available, R_1 of the projective measurement of energy based on the phase estimation algorithm $\mathcal{M}_{C_{U(t)}}$ is calculated according to Eq. (5.39) by

$$\begin{aligned} R_1(\mathcal{M}_{C_{U(t)}}|H) &= \max_k \sum_{1 > f_N \geq 0} P(2\pi f_N|\theta_k) (E(f_N) - E_k)^2 \\ &= \max_k \sum_{1 > f_N \geq 0} \frac{P(2\pi f_N|\theta_k)}{t^2} (E(f_N)t - E_k t)^2. \end{aligned} \quad (5.53)$$

We define an open ball $\mathcal{B}_k = \mathcal{B}(E_k t/2\pi, \sqrt{\varepsilon}t/2\pi)$ whose center and radius are given by $E_k t/2\pi$ and $\sqrt{\varepsilon}t/2\pi$, respectively. We rewrite Eq. (5.53) as

$$R_1(\mathcal{M}_{C_{U(t)}}|H) = \max_k \left(\sum_{f_N \in \mathcal{B}_k} + \sum_{f_N \notin \mathcal{B}_k} \right) \frac{P(2\pi f_N|\theta_k)}{t^2} (E(f_N)t - E_k t)^2. \quad (5.54)$$

We bound the two terms of the right-hand side of this equation. The first term is bounded by

$$\sum_{f_N \in \mathcal{B}_k} \frac{P(2\pi f_N|\theta_k)}{t^2} (E(f_N)t - E_k t)^2 \leq \varepsilon \sum_{f_N \in \mathcal{B}_k} P(2\pi f_N|\theta_k) \leq \varepsilon. \quad (5.55)$$

The first inequality is derived from the definition of \mathcal{B}_k and the second inequality is derived from the property of the probability distribution. The other term is

bounded as

$$\sum_{f_N \notin \mathcal{B}_k} \frac{P(2\pi f_N | \theta_k)}{t^2} (E(f_N) - E_i t)^2 \leq \sum_{f_N \notin \mathcal{B}_k} \frac{4\pi^2}{t^2} \left(\frac{\sin 2^N (\theta_k - 2\pi f_N) / 2}{2^N \sin (\theta_k - f_N) / 2} \right)^2 \quad (5.56)$$

$$\leq \sum_{f_N \notin \mathcal{B}_k} \frac{4\pi^2}{t^2} \frac{1}{2^{2N} \sin^2 (\theta_k - f_N) / 2} \quad (5.57)$$

$$\leq \frac{1}{t^2} \frac{4\pi^2}{2^N \sin^2 \sqrt{\varepsilon} t} \quad (5.58)$$

$$\leq \frac{16\pi^2}{2^N \varepsilon t^4}, \quad (5.59)$$

where the first inequality is derived from $\Delta_{\max} t < 2\pi$ and the third from the fact that the total number of outcomes f_N is 2^N . Combining these two results, we obtain

$$R_1(\mathcal{M}_{C_{U(t)}} | H) \leq \varepsilon + \frac{16\pi^2}{2^N \varepsilon t^4}. \quad (5.60)$$

On the other hand, R_2 of \mathcal{M}_{PEA} is calculated by

$$R_2(\mathcal{M}_{C_{U(t)}} | H) = 0, \quad (5.61)$$

since the total unitary matrix according to this algorithm commutes with the local Hamiltonian of the target system. For the same reason, we obtain

$$R_2(\mathcal{M}_{PEA} | \tilde{H}) = 0. \quad (5.62)$$

5.6 Evaluating the running time

We regard the running time of the algorithm as the total calling time of the Hamiltonian dynamics under the assumption that the quantum computer can operate in a time scale much father than that of the Hamiltonian dynamics of the target system.

For given Δ_{\max} and $\varepsilon \in (0, 1]$, we calculate the total running time T_{PE} i.e., the total calling time of the Hamiltonian dynamics to obtain

$$R_1(\mathcal{M}_{PEA} | \tilde{H}) \leq 3\varepsilon. \quad (5.63)$$

First, choose t so that $\Delta_{\max} t \leq \pi/2$. Next, choose N so that the second term of Eq. (5.60) is equal to ε , which implies that $2^N = O((\Delta_{\max})^4 / \varepsilon^2)$. Finally, choose m according to Eq. (5.46), so that the second term in Eq. (5.60) is bounded as

$$\frac{2^N (2\delta) 4\pi^2}{t^2} \leq \varepsilon. \quad (5.64)$$

The total running time is given by

$$T_{PE} = (2^{N+1} - 1) \times m \times \frac{t}{m}. \quad (5.65)$$

All in all, to achieve Eq. (5.63) requires

$$T_{PE} = O\left(\frac{(\Delta_{\max})^3}{\varepsilon^2}\right). \quad (5.66)$$

Thus the running time of our method based on phase estimation and universal controllization does not depend on the dimension of the system d , whereas the running time of the tomography-based method depends on d^4 to achieve the same performance as the projective measurement of energy.

Chapter 6

Conclusion

The results in this thesis is summarized as follows.

1. To evaluate the performance of implemented projective measurements of energy, we formulate two evaluation functions called *fluctuation of measurement value* and *non-repeatability*, which can evaluate how much a measurement is different from the ideal projective measurement of an observable. The fluctuation of measurement value is defined as the mean squared error of the measurement outcome. Non-repeatability evaluates how a measurement behaves differently from the repeatable hypothesis. We formulate two relations between the known evaluation methods and ours. One relationship is that the fluctuation of measurement value and non-repeatability give an upper bound of the Monge distance between two measurements. The other is, when the fluctuation of measurement value is zero, the diamond norm of between measurement instruments becomes well-defined and the value becomes the same as the non-repeatability.
2. We construct an implementation method of projective measurement of energy via a linear estimation scheme of a unitary operation (tomography based method) which is suggested in the paper of Aharonov et. al. (2002). We first formulate the linear estimation scheme of unitary evolution. We analyze efficiency of this method on the assumption that there is an appropriate converter which deforms a given operator into a regular, normal matrix while leaving the statistical property of each element the same as the original operator. We calculate a sufficient time to guarantee the fluctuation of measurement value below some small value ε . We find that the tomography based method takes the time proportional to $O(d^4 \Delta_{\max} / \varepsilon)$, where d is the dimension of the target system and Δ_{\max} is the difference between the largest energy eigenvalue and the smallest energy eigenvalue. We also calculate the non-repeatability for the tomography based method. We found that there is a case that the non-repeatability of the tomography based method cannot converge to zero even in the limit of infinite measurement time.
3. We construct a new quantum randomized algorithm, universal controllization which approximately achieves the controlled Hamiltonian dynamics avoiding the impossibility of exact implementation. In our new algorithm, the Hamilton dynamics is divided into a sequence of short time segments and randomization processes are inserted between sequences. The randomized dynamics decouples emerging entanglement between the target system

and the quantum computer which has the main obstacle for controllization of the unknown Hamiltonian.

4. We present a phase estimation based method, which utilizes the Hamiltonian dynamics of the system as a resource for the quantum algorithm, and construct the projective measurement of energy on the system without identifying all parameters of the Hamiltonian. The phase estimation based method is implemented via the universal controllization scheme. We calculate a sufficient time to guarantee the fluctuation of measurement value below some small value ε . We find that the phase estimation based method takes time proportional to $O(\Delta_{\max}^3/\varepsilon^2)$. We also calculate the non-repeatability and found that the non-repeatability of the phase estimation based method is always zero for any amount of measurement time consumed.

From these results, we conclude the following properties about the accuracy and efficiency for performing projective measurement of energy. When the fluctuation of measurement value is smaller than $O(\Delta_{\max}^2/d^4)$, the tomography based method is more efficient than the phase estimation based method. However, the dimension of a physical system grows exponentially with the system size given by the number of constituent particles whereas Δ_{\max} grows only linearly when we assume nearest neighbor interactions between particles, which is frequently encountered in physics. On non-repeatability, our phase estimation based method shows the same performance as the ideal projective measurement of energy, nevertheless the tomography-based scheme can not guarantee the small amount of the value. Therefore, as for the fluctuation of measurement value, our phase estimation based method shows better performance than the tomography based method when the system size is sufficiently large. The projective measurement of energy expected to be useful in applications for metrology breaking the standard quantum limit (quantum non-demolition measurement) and for the experimental confirmation of the fluctuation theorems in non-equilibrium quantum systems. For metrology, larger size systems have higher sensitivity to detect small deviation caused by an extremal source, e.g. the gravity wave. The experimental confirmation of fluctuation theorems on large quantum systems is also important to test whether these theories are the origin of the thermodynamics or not. The study in this thesis suggests that the straight-forward method (tomography based method) is inefficient for scaling the system size suitable for these applications, and offers another efficient quantum algorithm.

In the field quantum information the theory of *super-map*, what types of quantum operations become possible by combine given unitary operations and quan-

tum operations independent of the unitary operations have been interested in recent years. The study of seeking computational power using a root of a given unitary gate has been also actively studied as the *fractional query problem* in these days. These problems correspond to the case that we can utilize a Hamiltonian dynamics of a system, which is a standard condition in quantum physics. Thus the many these developments in quantum information going to be useful tools in physics. However we note that there are gaps in terminology and precondition between two fields, and it often be obstacles for linking them. In this thesis, we made a formulation of the measurement which can treat measurements in both standard physics and quantum information. As the result, we utilize the fruitful algorithm developed in quantum information for the measurement which provides a fundamental property for understanding physics. Inversely, the idea developed in quantum physics, dynamical decoupling, also provides a hint to establish a super-map, controllization, approximately available which was known to be impossible in quantum information. The more we understand the connection between two fields, the more understanding of quantum physics or unexpectable quantum algorithms are to be found.

Acknowledgments

My deepest appreciation goes to my supervisor, Mio Murao, for her great help. Throughout my post graduate course, she always pointed me to the relevant questions of my research and provided me many valuable opportunities. I'm also very grateful for all the time (including her holidays) she spent for correcting my writings and giving me precious advise. I owe her much. I also owe much to my coworker, Akihito Soeda. He patiently helped me to bring my cluttered ideas to understandable formulations. The results presented in this thesis wouldn't have been possible without him.

I would like to express my great appreciation to the chief examiner of my thesis Masahito Ueda for guiding me in everything. I'm also graterul to my examiner Masato Koashi giving precious advice on the technical part of my thesis. I would further like to thanks the other examiners, Izumi Tsutsui, Akira Shimizu, Masaki Ando for their valuable comments to me.

I am grateful to Professor Hroshi Imai and his group for their frequent support over the last 5 years. Their support has given me precious opportunities to present my study abroad.

I would also like to express my gratitude to Takanori Sugiyama and Yoshifumi Nakata for taking care of all concerns of my study life. Furthermore, I greatly appreciate the help from Peter S. Turner, Michal Hajdusek and Fabian Furrer in correcting my English writing and for cheering me up. I spent enjoyable time in my postgraduate terms with Eyuri Wakakuwa, Seiseki Akibue, Kosuke Nakago, Jisho Miyazaki, Kotaro Kato, Yuki Mori and Atsushi Shimbo by having discussions, teaching each other and joking around. I thank them a lot. I acknowledge the continuous, helpful support from Yuki Amano and Yumiko Wada in office works.

This work was supported by the Project for Developing Innovation Systems of MEXT, Japan and KAKENHI (Grant No. 23540463) of the Japan Society for the Promotion of Science.

Finally, I would like to express my heartfelt appreciation to my parents and my family. My life so far has been supported totally by their understanding,

kindness and generosity. I will never forget the importance of what I received from them and their blessing. At the last, I would like to add my sincere gratitude to my partner Ami Ito for how she is. You were my emotional support while writing this thesis.

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