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Doctoral Thesis

Study on real and imaginary time dynamical effects in quantum and classical systems

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The present thesis investigates two topics on the real- and imaginary-time dynamical effects of quantum systems, inspired by quantum annealing. The first topic is the quantum speed limit and the analysis is intended to show that the quantum speed limit is not a purely quantum phenomenon but a universal dynamical property of the Hilbert space. The second topic is exactness of the static approximation, and the analysis aims to solve the partition function of mean-field quantum spin systems exactly.

The quantum speed limit (QSL) describes the fundamental maximum rate for quantum time evolution. Since QSL originally developed in a similar context to Heisenberg's uncertainty principle, QSL has been considered a purely quantum phenomenon with no corresponding concept in classical mechanics. Recent studies have implied that QSL vanishes in the classical limit, and the time evolution of classical mechanics has no fundamental speed limit. However, in the present thesis, we show that a fundamental speed limit exists even in classical mechanics. As a result, we concluded that QSL is not a particular phenomenon to quantum mechanics; instead, QSL is a universal property of the time evolution of the Hilbert space.

Mean-field quantum spin systems are one of the simplest quantum spin models. Using the Suzuki-Trotter decomposition, a mean-field quantum spin system can be mapped on to a mean-field classical spin system which has the imaginary-time dependence. Since it is very difficult to explicitly treat the imaginary-time dependence of the partition function, we usually neglect the imaginary-time dynamical effect, which is called the static approximation. Although the static approximation is not necessarily exact for mean-field quantum spin systems, there is no general understanding of when the static approximation is exact, that is, mean-field quantum spin systems have not been shown to be solved exactly. In the present thesis, using the optimal control theory, we show that the static approximation is exact for a wide class of mean-field quantum spin systems, which is the first systematic result on the exactness of the static approximation.

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1. Introduction

This thesis studies the properties of real and imaginary time quantum systems from the view point of quantum annealing. Especially, we focus on mean-field quantum spin systems and the quantum speed limit. We start with a review of some topic on quantum dynamics, quantum annealing, quantum speed limit, and mean-field quantum spin systems in order to show the motivation of this thesis. In section 1.2, we explain quantum annealing as an approach from physics to combinatorial optimization problems. We describe the standing position of mean-field quantum spin systems in quantum annealing in Sec. 1.3. Section 1.4 introduces the quantum speed limit.

1.1. Time-dependent systems

When we first learn quantum mechanics, we explore the time-independent static property. In the time-independent Schrödinger equation, the purpose is to obtain the eigenstates and the eigenenergies, and even if these are known, all the static properties can be predicted in principle. Needless to say, this procedure is a very difficult problem in general.

However, the world we live in is dynamic, and it is a natural desire to explore the nature of time-dependent systems. In time-dependent quantum systems, the time dependent Schrödinger equation describes all of the system properties,

$$i\frac{d}{dt}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle \quad (1.1)$$

If we use the Magnus expansion [1], we can formally write the solution as follows,

$$|\psi(\tau)\rangle = U_\tau|\psi(0)\rangle \quad (1.2)$$

$$U_\tau = \exp\left(-\frac{i}{\hbar}\Omega_\tau\right), \quad (1.3)$$

$$\Omega_\tau = \int_0^\tau dt_1 H_{t_1} - \frac{i}{2\hbar} \int_0^\tau dt_1 \int_0^{t_1} dt_2 [H_{t_1}, H_{t_2}] + \dots \quad (1.4)$$

However, the Magnus expansion has an infinite order expansion and the difficulty of the problem has not changed. There are only a few examples where solutions of

time-dependent problems are obtained in a compact form, and it is very difficult to treat time-dependent problems in quantum systems. As a few solvable systems, the Landau-Zener model [2, 3] is a very famous time-dependent problem,

$$\hat{H}(t) = \frac{v}{2}t\hat{\sigma}^z + \Delta\hat{\sigma}^x. \quad (1.5)$$

When the system develops from $t = -\infty$ to $t = \infty$, the transition probability from the ground state to the first excited state is given by the closed compact form $\exp(-2\pi\Delta^2/v)$. However, when the time evolution is finite, the transition probability is expressed in a very complicated form using special functions. Solving a time dependent problem in finite duration is formidable task even for the simple two level system, not to mention many body systems.

1.2. Combinatorial optimization problems and Quantum annealing

In general, it is very difficult to solve time-dependent problems. Conversely, in order to solve combinatorial optimization problems [4, 5], quantum annealing [6] actively utilizes quantum dynamics. Combinatorial optimization problems represented by the traveling salesman problem appear in various fields in the real world [7], and it is socially very important to obtain the optimal solution (see appendix A.1 for combinatorial optimization problems). Interestingly, the problem of finding the optimal solution of combinatorial optimization problems can be reduced to the problem of obtaining the ground state of the classical spin system [8–10] (see appendix A.2.1 for example). Quantum annealing is a computational method for exploring the ground state of classical Ising spin systems by skillfully using quantum fluctuations, and is originally inspired by simulated annealing [11] (see appendix A.3 for simulated annealing). While simulated annealing gradually lowers the virtual temperature from high temperature to low temperature on a classical computer and searches for the ground state of classical spin systems by thermal fluctuation, quantum annealing searches the ground state by the tunneling effect of quantum fluctuations by gradually lowering quantum fluctuations as shown in Fig. 1.1.

The most important difference between simulated annealing and quantum annealing is that quantum annealing uses a natural physical phenomenon, the

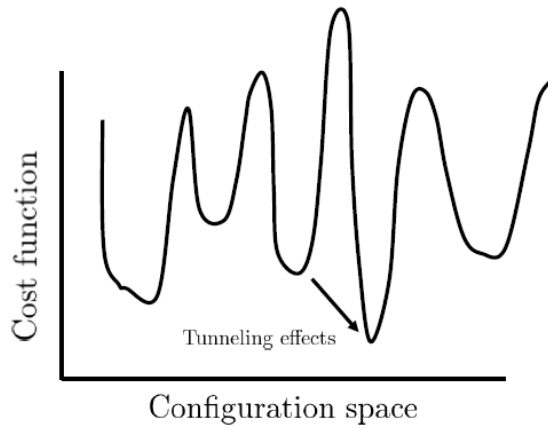


Figure 1.1.: A schematic view of quantum annealing. Quantum fluctuations search for the optimal solution

Schrödinger equation, whereas simulated annealing is a numerical calculation method on a classical computer.

The procedure of quantum annealing is constructed as follows. First, we prepare the driver Hamiltonian, which plays the role of quantum fluctuations, and the target Hamiltonian, which has the ground state corresponding to the optimal solution of the combinatorial optimization problem. At the initial time, the influence of quantum fluctuations is sufficiently strong. Next, we gradually weaken quantum fluctuations and strengthen the target Hamiltonian. Quantum fluctuations induce transitions of the state with time evolution of the Schrödinger equation and search the ground state of the target Hamiltonian. Finally, we completely eliminate the quantum fluctuation and obtain the eigenstate of the target Hamiltonian. If the state of the system develops properly, it is expected that the final state is close to the target ground state, which is the concept of quantum annealing.

Quantum annealing is closely related to adiabatic quantum computation [12,13] and is equivalent to adiabatic quantum computation when time evolution is limited to the adiabatic time evolution. Adiabatic quantum computation is a method of finding the ground state of the target Hamiltonian based on the adiabatic theorem [14]. The state of the system starts from an obvious ground state and follows

the instantaneous ground state of the system. As the result, we obtain the target ground state at the final time. Then, from the adiabatic theorem, the computational time of adiabatic quantum computation is proportional to the square inverse of the energy gap between the ground state and the first-excited state. Theoretically, it is known that the computational power of adiabatic quantum computation is equivalent to that of quantum circuit model [15, 16].

In quantum annealing, time evolution is not necessarily restricted to the adiabatic time evolution and quantum annealing is a concept including adiabatic quantum computation. However, in this thesis, we identify them mostly.

The computational time of adiabatic quantum computation reflects the quantum phase transition, because, in general, the quantum phase transition occurs in the process of quantum annealing reflecting the change of the ground state and the energy gap approaches to 0 rapidly [17]. Thus, the quantum phase transition strongly affects the efficiency of adiabatic quantum computation.

Finally, we mention the D-Wave machine. Quantum annealing has attracted much attention in recent years due to the physical implementation by the D-Wave machine [18, 19]. In the D-wave machine, thousands of qubits are implemented. However, coupling between spins can not be handled freely and is limited to local interactions. In addition, since the coherence time can not be taken long enough in the D-Wave machine, the adiabatic time evolution has not been realized and the effect of interaction with the thermal bath can not be ignored. Furthermore, only the transverse field is used as quantum fluctuation, and it is considered that its computational power is weaker than adiabatic quantum computation. Research to evaluate the performance of the D-Wave machine is still continuing. Recently, the D-Wave machine has been used as a quantum simulation, and the three-dimensional transverse field spin glass model and the Kosterlitz-Thouless transition transition have been observed [20, 21].

1.3. Mean-field quantum spin systems and imaginary-time dynamics

Research on the quantum phase transition of the quantum spin system is very important from the viewpoint not only of statistical mechanics but also of quantum annealing because the computational time of adiabatic quantum computation is strongly affected by the quantum phase transition. However, it is very difficult to analyze large quantum spin systems in general. This difficulty is the same as in

the spin systems in which the combinatorial optimization problems are mapped. Then, in order to analyze a large size quantum system and to investigate what kind of quantum fluctuation is effective for quantum annealing, there are many studies on mean-field quantum spin systems [22–31] because it is easier to calculate the thermodynamics limit [17]. Although mean-field quantum spin systems are simple models and do not directly reflect the nature of the real optimization problem, many works have been studying mean-field quantum spin systems as a touchstone for evaluating the performance of quantum annealing. Recent studies [23, 25, 29] showed that, through analysis of mean-field quantum spin system, inhomogeneous transverse field and non-stoquastic Hamiltonians [33–36] have a positive influence on the efficiency of quantum annealing, which are important concept of quantum annealing.

So far, we have introduced mean-field quantum spin systems from the viewpoint of adiabatic quantum computation. Indeed, dynamical problems are hidden in obtaining the partition function of mean-field quantum spin systems. When we analyze the partition function of mean-field quantum spin systems, the Suzuki-Trotter decomposition [32] which maps quantum system to classical system is used in general. At this time, although the partition function is represented by the order parameters similarly to mean-field classical systems. The difference from mean-field classical spin systems [4] is that the order parameters depend on the imaginary-time direction. Due to the imaginary-time dependence, it is very difficult to solve the partition function of mean-field quantum spin systems, and previous studies have used the static approximation [37] which neglects the imaginary-time dependence of the order parameters. Thus, mean-field quantum spins systems have not been solved exactly although they are one of the simplest quantum spin systems.

1.4. Quantum speed limit

We have focused on adiabatic quantum computation and the nature of the static system because it is very difficult to treat time-dependent problems. In contrast, can we impose some constraints on general time evolution? For example, in the theory of relativity, the speed of objects can not exceed the speed of light. Is there a fundamental limit also in time evolution of quantum mechanics? Although it is fundamentally different from the theory of relativity, there is an inequality called the quantum speed limit [38, 39], which gives an upper bound on the speed of

quantum time evolution. The quantum speed limit was originally developed in the context of time and energy uncertainty principle and is called the energy-time uncertainty relation. The quantum speed limit is also applied to quantum annealing and gives us the usual conclusion that it is impossible to infinitely shorten the computational time of quantum annealing [40, 41].

Since the quantum speed limit appeared in the context of the uncertainty principle, the quantum speed limit has been regarded as a purely quantum phenomenon in the previous studies. Recent previous studies [42–45] argued that the quantum speed limit disappears at the classical limit. However, as a question, is there a limitation to simulated annealing which is a classical algorithm corresponding to quantum annealing?

1.5. Outline

The goal of this thesis is to deepen the understanding of dynamics, motivated by quantum annealing. We especially focus on two topics.

The first topic is on the dynamics of the imaginary time Schrödinger equation that appears in the process of exactly solving mean-field quantum spin systems. Although exact analysis of mean-field quantum spin systems is also very important from the viewpoint of quantum annealing, the order-parameters depend on imaginary-time due to the Suzuki-Trotter decomposition, and mean-field quantum spin systems have not been solved exactly without the static approximation [37], which means that there is no absolutely reliable result for mean-field quantum spin systems. Then, we have to establish the precise theory for understanding the nature of the critical phenomena. In this thesis, we solve this problem for a wider class of mean-field quantum spin systems, by regarding the problem of solving the partition function as the optimal control problem in the imaginary time Schrödinger equation. The optimal control problem is the problem of determining the time dependence of the coefficients of differential equations so as to maximize the given cost function. According to the optimal control theory [46, 47], in order to solve the optimal control problem, it is necessary to solve the equations of motion of the corresponding classical Hamiltonian for special initial and terminal conditions. As a result, we prove that the static approximation gives the exact solution for a wider class of mean-field quantum spin systems. Our method is the first technique to deal with mean-field quantum spin systems exactly and systematically. Furthermore, our result is also interesting from the

view point of classical nonlinear integrable system. The classical Hamiltonian equations corresponding to mean-field quantum spin systems treated in this thesis has nonlinearity. Although the classical Hamiltonian with nonlinearity usually belongs to nonintegrable system, it is quite interesting that we can show that the classical Hamiltonians treated in this thesis belong to integrable system, that is, the classical Hamiltonians corresponding to mean-field quantum spin systems belong to classical nonlinear integrable system. Our model does not seem to be included in the Toda lattice [48] and the Toda hierarchy [49] which are the most famous classical nonlinear integrable system of finite degrees of freedom. It is an interesting future problem to clarify whether our classical Hamiltonian systems are included in classical nonlinear integrable system known in the previous studies.

The second topic is to extend the quantum speed limit to classical systems. Previous studies [42–45] so far have suggested that the quantum speed limit is a phenomenon particular to quantum systems. However, we notice that quantum nature such as non-commutativity is not used at all for deriving the quantum speed limit. Then, we clarify that similar speed limits also exist in classical systems, such as the classical Liouville equation and the imaginary-time Schrödinger equation which is equivalent to the Fokker-Planck equation and the classical master equation. Our result concludes that it is also impossible to infinitely shorten the computational time of simulated annealing similarly to quantum annealing, which is a natural consequence.

Let us overview the present thesis. Chapter 2 summarizes the necessary background knowledge. We first describe the framework of quantum annealing and adiabatic quantum computation. After that, we explain the relation between adiabatic quantum computation and quantum phase transition and clarify the role of mean-field quantum spin systems in the context of adiabatic quantum computation. After the concept of the static approximation, which plays a very important role in mean-field quantum spin systems, is introduced, we emphasize that mean-field quantum spin systems have not been solved exactly. Next, we introduce the Grover problem in adiabatic quantum computation. The Grover problem [50] is a famous problem in which quantum acceleration is realized. Moreover, we introduce the quantum speed limit and explain the result of applying it to the Grover problem in quantum annealing.

Chapter 3 is the first main result of this thesis. Identifying the evaluation of the imaginary time dependence of mean-field quantum spin systems with the optimal control problem in the imaginary-time Schrödinger equation, we obtain exactly

the partition function of a wider class of mean-field quantum spin systems. First of all, we apply our method to the p -spin model with the transverse field which is the simplest mean-field quantum spin system. Solving the partition function exactly, we clarify that the static approximation is exact for this model. Next, we generalize our method to the generalized Hopfield model and show that the static approximation gives the exact solution for this model. We apply this result to quantum annealing and show that the analysis of previous studies in quantum annealing is exact. Furthermore, we extend our result to a wider class of mean-field quantum spins systems under certain conditions. Finally, we clarify that the classical Hamiltonians, which appeared through the optimal control problem, belong to classical nonlinear integrable system.

Chapter 4 explains the second main result of this thesis. We extend the quantum speed limit to classical systems. We first show that the classical Liouville equation has a speed limit similar to the quantum speed limit. Next, we show that the imaginary-time Schrödinger equation has also a similar speed limit. Besides, we obtain another type of the quantum speed limit and apply it to the Grover problem in imaginary-time quantum annealing. As the result, we prove that the optimal computational time of the Grover problem is order $\log M$ for the problem size M in imaginary-time quantum annealing.

We summarize our findings and conclude this thesis in Chap. 5.

2. Quantum annealing

This chapter is devoted to the necessary background knowledge and our motivation. First, Sec. 2.1 introduces quantum annealing and quantum adiabatic computation. Next, we explain the role of mean-field quantum spin systems in adiabatic quantum computation in Sec. 2.2. We emphasize that mean-field quantum spin systems have not been solved without the static approximation. Section 2.3 demonstrates that adiabatic quantum computation can solve the Grover problem by the computational time of the order \sqrt{M} for the problem size M while classical algorithms requires order M . In Sec. 2.4, we review the quantum speed limit. As an application to quantum annealing, it is shown that the optimal computational time of the Grover problem is bounded by \sqrt{M} . In addition, we note that the quantum speed limit has been regarded as a phenomenon particular to quantum systems.

2.1. Quantum annealing and adiabatic quantum computation

2.1.1. Quantum annealing

Let us introduce quantum annealing. We consider the time-dependent Hamiltonian $\hat{H}(t)$,

$$\hat{H}(t) = \Gamma(t)\hat{H}_I + \hat{H}_P, \quad (2.1)$$

where \hat{H}_I and \hat{H}_P are called the driver Hamiltonian and the target Hamiltonian, respectively. The ground state of $\hat{H}_I(t)$ is known and our purpose is to find the ground state of \hat{H}_P . $\hat{H}_I(t)$ plays a role of quantum fluctuation. At the initial time, $\Gamma(t)$ is sufficiently strong so that the initial state of the system is the trivial ground state of \hat{H}_I . By gradually weakening $\Gamma(t)$ and strengthening the influence of \hat{H}_P , time evolution of the state searches the ground state of \hat{H}_P . The system

follows the time-dependent Schrödinger equation,

$$i\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle. \quad (2.2)$$

To trigger state transitions, a necessary condition for \hat{H}_I is noncommutability with \hat{H}_P ,

$$[\hat{H}_P, \hat{H}_I] \neq 0. \quad (2.3)$$

If we slowly change the strength of \hat{H}_I closer to 0 with an appropriate schedule, the state will remain near the ground state at each instant, so that finally it is expected that the state of the system approaches the target ground state of \hat{H}_P . This is the principle of quantum annealing.

In quantum annealing, the homogeneous transverse field has been widely used as quantum fluctuation,

$$\hat{H}_I = -\sum_{i=1}^N \hat{\sigma}_i^z. \quad (2.4)$$

When the driver Hamiltonian \hat{H}_I is given by the homogeneous transverse field and the target Hamiltonian \hat{H}_P is given by classical Ising spin system

$$\hat{H}_P = -\sum_{i,j} J_{i,j} \hat{\sigma}_i^z \hat{\sigma}_j^z, \quad (2.5)$$

Morita and Nishimori [51] proved that the state always converges to the target ground state at the final time if we take the schedule of the transverse magnetic field as follows,

$$\Gamma(t) = a(\delta t + c)^{-1/(2N+1)}, \quad (2.6)$$

where a and c are constants not depending on N . We emphasize that this is the worst evaluation in the case of the transverse field.

Quantum fluctuation is not limited only to transverse field. Recently, as a driver Hamiltonian, inhomogeneous transverse field has been proposed and its effectiveness is being studied [29, 52–55],

$$\hat{H}_I \Rightarrow \hat{H}_I(t) = -\Gamma(t) \sum_{i=1}^{N(1-f(t))} \hat{\sigma}_i^x, \quad (2.7)$$

where $f(t)$ is a time-dependent function and represents the ratio of the transverse magnetic field applied. Furthermore, there is also a proposal [33, 34] to use the

nonstoquastic Hamiltonians as quantum fluctuations in which it is difficult to simulate quantum system with quantum Monte Carlo method. These will be explained in the next subsection.

Finally, as a precaution we note that adiabatic quantum computation is the time evolution of quantum annealing limited to the adiabatic time evolution and quantum annealing is a slight wider concept than adiabatic quantum computation. Quantum annealing does not necessarily consider adiabatic time evolution, and it is known that quantum acceleration can be realized against special problems by positively utilizing the transition between the ground state and the first excited state [56]. Nevertheless, the adiabatic time evolution is often considered in quantum annealing because it is theoretically very difficult to deal with general time dependent problems and it is proved that the computational power of adiabatic quantum computation is equivalent to that of quantum circuit model [15,16]. We note that, in this thesis, we identify quantum annealing as adiabatic quantum computation for simplicity.

2.1.2. Adiabatic quantum computation

Adiabatic quantum computation is a concept included in quantum annealing. In adiabatic quantum computation, time evolution is limited only to adiabatic time evolution. We consider the following time-dependent Hamiltonian,

$$\hat{H}(t) = f(t)\hat{H}_I + (1 - f(t))\hat{H}_P(t) \quad (2.8)$$

where the time-dependent function $f(t)$ satisfies the boundary condition $f(0) = 0$ and $f(\tau) = 1$. We start from the trivial ground state of \hat{H}_I . If the time evolution is sufficiently slow, the quantum adiabatic theorem guarantees that the state follows the instantaneous ground state of $\hat{H}(t)$ and the final state arrives at the target ground state \hat{H}_P at final time τ . The condition of adiabatic theorem is given as follows [14],

$$\frac{\left| \langle k(t) | \frac{\partial \hat{H}(t)}{\partial t} | n(t) \rangle \right|}{(E_k(t) - E_n(t))^2} \ll 1. \quad (2.9)$$

This inequality means that the time evolution should be slow in the region where the energy gap is small. In addition, the minimum value of the energy gap strongly influences the computational time of adiabatic quantum calculation. For example, in the Grover problem [50,57], using the adiabatic theorem positively, quantum acceleration of \sqrt{N} is realized (this is discussed in the next section.).

It is known that the computational power of adiabatic quantum computation is equivalent to quantum circuit model and it is possible for each other to simulate each other in polynomial overhead [15,16]. Adiabatic quantum computation has a characteristic that it is relatively strong against noise. It is also an advantage that there is no need to perform complicated gate operations. Instead, it is necessary to properly schedule the time evolution, such as a slow time evolution where the energy gap is close to 0. In addition, it is a difficult problem to know the region with a small energy gap. Furthermore, there is a major disadvantage that the theory of error correction has not been established, unlike the quantum circuit model. Once transition from the ground state to other excited states occurs, the computation fails. Although there are some studies on error correction of quantum annealing [27, 58–62], systematic error correction theory like that of quantum circuit model has not been found.

2.1.3. Adiabatic quantum computation and quantum phase transition

The computation time of adiabatic quantum computation is closely related to quantum phase transition. In adiabatic quantum computation, it is generally known that quantum phase transition occurs, reflecting a transition from a trivial ground state to a non-trivial ground state. Then, in a large system, because the energy gap rapidly approaches 0 at phase transition point, the computational time becomes very large. On the contrary, this means that the performance of quantum annealing can be evaluated by investigating statistical mechanical properties of the target Hamiltonian.

According to the finite-size scaling theory, when applied to a second order phase transition with a divergent correlation length, physical quantities generally behave polynomially as a function of the system size [17, 63, 64]. In contrast, the gap is expected to close exponentially fast at the first order quantum phase transition: the two ground states at opposite sides of the first order transition point have significantly different properties and consequently their overlap in a finite-size system is very – typically exponentially – small. The overlap of the two states determines the energy gap since the overlap corresponds to the off-diagonal elements of the effective two-level Hamiltonian describing the system around the transition point and the gap is directly related to the magnitude of the off-diagonal elements. It is therefore expected that the order of quantum phase transition in the thermodynamic limit is generally in one-to-one correspondence with the rate

of the gap closing toward the thermodynamic limit, polynomially for the second order transition and exponentially for the first order transition [65,66].

This rule by experience implies that adiabatic quantum computation is efficient when the second order phase transition occurs in the course of computation, while the first order phase transition signifies inefficiency of quantum annealing. Of course, this is only rule by experience, and there are a few special counterexamples [67–71]. However, it is believed that the above rule of experience is established in most cases.

2.2. Quantum annealing and mean-field quantum spin system

In general, it is very difficult to analyze quantum systems, and it is required to evaluate the performance of quantum annealing in a region with large system size. As mentioned earlier, although the computational time of adiabatic quantum computation reflects the property of quantum phase transition, it is a formidable task to diagonalize large size quantum spin systems. Then, for the purpose of investigating what kind of quantum fluctuation accelerates the efficiency of quantum annealing, there are some studies on mean-field quantum spin systems in the context of quantum annealing [22–31].

In this section, we explain a relation between quantum annealing and mean-field quantum spin systems. We also introduce "nonstoquastic" Hamiltonians [33–36], which is an important concept in quantum annealing, and the static approximation, which plays a important role in the analysis of mean-field quantum spin systems [37]. The goal of this section is to show that mean-field quantum spin systems have not been solved without the static approximation.

2.2.1. Mean-field model with transverse field

First, we start with the p -spin model with the transverse field which is one of the simplest mean-field quantum spin systems,

$$\hat{H} = -N \left(\frac{1}{N} \sum_{i=1}^N \hat{\sigma}_i^z \right)^p - \Gamma \sum_{i=1}^N \hat{\sigma}_i^x. \quad (2.10)$$

Jörg and *et al.* [22] evaluated the performance of quantum annealing with the transverse field as quantum fluctuation, based on the analysis of the phase diagram. Consider that quantum annealing is applied to this model. At the initial

time $t = 0$, the transverse field is strong enough and all spins point in the x direction. We gradually weaken the transverse field, and the transverse field vanishes and all spins point in the z direction at the final time $t = \tau$. Of course, the ground state of the final time is trivial. However, Ref. [22] shows that the first order phase transition occurs in the process of quantum annealing, which means that quantum annealing can not find the trivial ground state.

2.2.2. XX interaction and non-stoquastic Hamiltonians

Quantum annealing only with the transverse field can not efficiently solve the ground state of the p -spin model which is a simple problem. In order to overcome this difficulty and to investigate what kind of quantum fluctuation is efficient for quantum annealing, Seki and Nishimori [23] introduced XX interaction $N \left(\sum_{i=1}^N \hat{\sigma}_i^x / N \right)^2$,

$$\hat{H}(t) = -N \left(\frac{1}{N} \sum_{i=1}^N \hat{\sigma}_i^z \right)^p - \Gamma_1 \sum_{i=1}^N \hat{\sigma}_i^x + \Gamma_2 N \left(\frac{1}{N} \sum_{i=1}^N \hat{\sigma}_i^x \right)^2. \quad (2.11)$$

where we note $\Gamma_1 \geq 0$ and $\Gamma_2 \geq 0$. By analyzing the phase diagram for the parameters Γ_1 and Γ_2 , they showed that there are paths through secondary phase transition by avoiding the first order phase transition in the process of quantum annealing. This result means that, for the p -spin model, the computational time of quantum annealing is exponentially improved as compared with the case of only the transverse field. The XX interaction seems to be non-physical at first glance, and many people may wonder why it is introduced. Indeed, the XX interaction is closely related to the non-stoquastic Hamiltonians [33–36] which have attracted a lot of attention in the field of quantum annealing in recent years.

Here, we introduce the concept of non-stoquastic Hamiltonians. The definition of the non-stoquastic Hamiltonians is that the Hamiltonian has both positive and negative elements in the off-diagonal elements in the standard computational basis $|\hat{\sigma}^z\rangle$ [33]. Then, the non-stoquastic Hamiltonians can not be simulated efficiently in classical computers because the negative sign problem emerges in quantum Monte Carlo method [72]. Interestingly, while the computational power of quantum annealing is equivalent to that of quantum circuit model when allowing the existence of general non-stoquastic Hamiltonians, adiabatic quantum computation only with the transverse field does not have the same computing power as quantum circuit model [15, 16]. Therefore, it is considered that the non-stoquastic Hamiltonians induce essential quantum effect and speed up the calculation for adiabatic quantum computation.

For the above reasons, the performance evaluation of quantum annealing in the case where the non-stoquastic Hamiltonian is addressed attracts recently a great deal of attention. Interestingly, introducing XX interaction into the p -spin model with transverse field leads to a negative sign problem on the z basis when $\Gamma_1 \geq 0$ and $\Gamma_2 \geq 0$; the XX interaction is a non-stoquastic Hamiltonian. Nishimori and Takada [34] argued that the introduction of XX interaction has intrinsic quantum effects on the p -spin model.

Seki and Nishimori [25] also analyzed the Hopfield model that complicates the p -spin model,

$$\hat{H} = -N \sum_{\mu=1}^k \left(\frac{1}{N} \sum_{i=1}^N J_i^\mu \hat{\sigma}_i^z \right)^p - \Gamma_1 \sum_{i=1}^N \hat{\sigma}_i^x + \Gamma_2 N \left(\frac{1}{N} \sum_{i=1}^N \hat{\sigma}_i^x \right)^2, \quad (2.12)$$

where $\Gamma_1, \Gamma_2 \geq 0$, p is an integer denoting the degree of interactions, and k is an integer representing the number embedded pattern and J_i^μ takes ± 1 at random. They found that there are paths through the second order phase transition by avoiding the first order phase transition by the XX interaction when the number of patterns is finite.

Of course, mean-field models are simple models, and the XX interaction is not necessarily effective for general models. However, their analysis is a very interesting result in that it is shown analytically that non-stoquastic Hamiltonian accelerates quantum annealing as compared with the case of the transverse field. In addition, since mapping realistic combination problems to Ising models often results in long-range interaction, analysis of mean-field models is not necessarily meaningless.

Recently, slightly modified quantum Monte Carlo method [36] has been proposed only for all connected XX interaction $N \left(\sum_{i=1}^N \hat{\sigma}_i^x / N \right)^2$. It is necessary to further study whether this method can really simulate all connected XX interaction efficiently. What kind of non-stoquastic Hamiltonians is effective for quantum annealing is still being studied [73–75].

2.2.3. Inhomogeneous transverse field

Although we have considered the homogenous transverse field so far, D-Wave machine has recently implemented the function to locally change the strength of the transverse field, and has found examples where the efficiency of quantum annealing is improved compared to the case of only transverse field [55]. Theoretically, numerical calculations of one-dimensional systems have showed that inhomogeneous transverse field improves the efficiency of quantum annealing compared

only with homogeneous transverse field [52–54]. As it is still possible to realize inhomogeneous transverse field on the actual machine, quantum annealing of inhomogeneous transverse field has recently been attracting interest.

Performance evaluation of inhomogeneous transverse field in quantum annealing is also analyzed for mean field models.

$$\hat{H} = -N \left(\frac{1}{N} \sum_i \hat{\sigma}_i^z \right)^p - \sum_i h_i \hat{\sigma}_i^z - \sum_i \Gamma_i \hat{\sigma}_i^x, \quad (2.13)$$

where h_i follows the Gaussian distribution with an average of 0 or the binary distribution $h_i = \pm h_0$. Susa and *et al.* [29] analyzed the phase diagram and found that, when inhomogeneous transverse field is addressed, there are paths avoiding the first order phase transition at absolute zero temperature, that is, inhomogeneous transverse field accelerates quantum annealing exponentially for the above mean-field model compared only with transverse field. They also analyze the phase diagrams at finite temperature because experimental systems have finite low temperature [31]. It is shown that, although it is impossible to avoid the first order phase transition at finite temperature, the exponential decreasing rate of the energy gap with respect to the system size N weakens and quantitatively accelerates the efficiency of quantum annealing with inhomogeneous transverse field.

Theoretically, it is not clarified why inhomogeneous transverse field is effective as compared with homogeneous transverse field, as one picture, Susa and *et al.* stated "*One of the possibilities may be that a phase transition is a cooperative phenomenon involving all degrees of freedom, and inhomogeneity of the field would jeopardize the cooperation between different parts of the system. If this crude picture captures some of the essential features of the present scheme, a similar phenomenon might be observed in more complex systems, such as spin glasses with finite connectivity (e.g., in finite spatial dimensions). It would be worth the effort to study many other cases.*".

Although quantum annealing of inhomogeneous transverse field is not universal quantum computation, it is sufficiently meaningful to study for practical use because the actual machine is restricted.

2.2.4. Static approximation and imaginary-time dynamics

We have introduced the analysis of mean-field quantum spin systems and omitted the details of the analysis. One may think that it is easy to obtain the partition function of mean-field quantum spin systems exactly because mean-field classical spin systems can be easily solved by the saddle point method when there is no

randomness [17]. Rather, it is a difficult problem to solve mean-field quantum spin systems exactly. In fact, the analysis of the previous section is not necessarily exact and they are based on an approximation, which is called the static approximation [37]. In the following, we will explain the static approximation.

When we solve mean-field quantum spin systems, we map the partition function to that of the classical system by the Suzuki-Trotter decomposition [32]. The Suzuki-Trotter decomposition is a method of dividing the exponential matrix of two non-commutative matrices \hat{A} and \hat{B} in order to calculate the partition function of quantum systems,

$$e^{\hat{A}+\hat{B}} = \lim_{M \rightarrow \infty} \left(e^{\hat{A}/M} e^{\hat{B}/M} \right)^M, \quad (2.14)$$

where M is called the Trotter number. The above decomposition is mathematically rigorous in the limit of $M \rightarrow \infty$. Then, it is possible to treat \hat{A} and \hat{B} separately in exchange for the fact that an infinite number of products are generated.

For example, we re-consider one of the simplest mean-field quantum spin systems, the p -spin model with the transverse field (2.10). For $\Gamma = 0$, the partition function of the classical p -spin model can be represented by one ordered parameter m ,

$$Z = \int dm e^{-N(p-1)\beta m^p} \left\{ \text{Tr} \left(e^{\beta p(m)^{p-1} \hat{\sigma}^z} \right) \right\}^N. \quad (2.15)$$

However, for $\Gamma \neq 0$, the order parameters of the partition function depend on the imaginary-time variable due to the Suzuki-Trotter decomposition. The partition function is given by

$$Z = \lim_{M \rightarrow \infty} \left(\prod_{t=1}^M \int dm^z(t) \right) e^{-N(p-1) \frac{\beta}{M} \sum_{t=1}^M (m^z(t))^p} \left\{ \text{Tr} \left(\prod_{t=1}^M e^{\frac{\beta}{M} p(m^z(t))^{p-1} \hat{\sigma}^z} e^{\frac{\beta}{M} \Gamma \hat{\sigma}^x} \right) \right\}^N, \quad (2.16)$$

where $m^z(t)$ is the order parameter, M denotes the Trotter number and t is the index of the Trotter number. Since $m^z(t)$ depends of the imaginary time t , the partition function is expressed by the sum of all possible integral paths for $m^z(t)$ and it is very difficult to treat the trace exactly. Most previous studies assume that, in the thermodynamic limit $N \rightarrow \infty$, the static path $m^z(t) = \text{const.}$ only contributes to the partition function and neglect the imaginary-time dependence of $m^z(t)$, which is called the static approximation [37]. When we use the static

approximation, we can obtain the free energy and the self-consistent equation,

$$f_{\text{SA}} = (p-1)(m^z)^p - \frac{1}{\beta} \log \left\{ 2 \cosh \left(\beta \sqrt{p^2(m^z)^{2p-2} + \Gamma^2} \right) \right\}, \quad (2.17)$$

$$m^z = p(m^z)^{p-1} \frac{\tanh \left(\beta \sqrt{p^2(m^z)^{2p-2} + \Gamma^2} \right)}{\sqrt{p^2(m^z)^{2p-2} + \Gamma^2}}. \quad (2.18)$$

Based on these equations, previous studies investigated the property of the phase diagram [22–31].

The static approximation is the first-order approximation to study analytically mean-field quantum spin systems and has been applied to various models. However, the static approximation does not necessarily give a good approximate solution.

For the p -spin model treated in previous section (2.10), (2.11) and (2.13), numerical calculation and other analytical calculations support the validity of the static approximation [22, 23, 25, 26, 29].

On the other hand, for the p -spin interacting spin-glass model which has the spin-glass phase,

$$\hat{H} = - \sum_{i_1 < \dots < i_p} J_{i_1 \dots i_p} \hat{\sigma}_{i_1}^z \dots \hat{\sigma}_{i_p}^z - \Gamma \sum_i \hat{\sigma}_i^x, \quad (2.19)$$

$$P(J_{i_1 \dots i_p}) = \left(\frac{N^{p-1}}{J^2 \pi p!} \right)^{1/2} \exp \left\{ - \frac{N^{p-1}}{J^2 p!} \left(J_{i_1 \dots i_p} - \frac{j_0 p!}{N^{p-1}} \right)^2 \right\}, \quad (2.20)$$

it is known that the static approximation gives a non-physical solution [76–84] because the entropy of the paramagnetic phase has finite values in the low temperature limit.

In addition, in the Hopfield model (2.12), it is unclear whether the static approximation is exact or not. Although Nishimori and Nonomura [85] predicted that the static approximation is exact for finite-number patterns and can be broken for infinite-number patterns, it is an unsolved problem.

Based on these previous studies, we investigate the exactness of the static approximation for mean-field quantum spin systems in Chap. 3. We regard the imaginary time dependence of the partition function as the result of time evolution of the imaginary-time Schrödinger equation [86, 87], and clarify that the problem of exactly obtaining the partition function is equivalent to the dynamical problem which belongs to the optimal control problem. Then, using the optimal control theory [46, 47], we solve the optimal control problem exactly and show that the static approximation is exact for a wider class of mean-field quantum spin systems including the Hopfield model with finite-number patterns.

2.3. Grover problem and adiabatic quantum computation

So far we have discussed the relation between adiabatic quantum computation and mean-field quantum spin systems. Theoretically, adiabatic quantum computing has the computing capacity equivalent to quantum circuit model [15, 16]. Here, we will explain how the problem of quantum acceleration realized by quantum circuit model is obtained by adiabatic quantum computation.

The Grover problem is a very famous problem where quantum acceleration is realized by quantum circuit model [50]. The Grover problem is also called database search problem, and it is a problem of finding one correct answer out of M possibilities. Because of the need to search for answers one by one, the computational complexity of classical algorithms is naturally of order M . On the other hand, in quantum circuit model, Grover [50] discovered an algorithm that can find an answer with the computational complexity of order \sqrt{M} . Then, there is a natural question whether adiabatic quantum computation can solve the Grover problem by order \sqrt{M} computation. In the following, we will formulate the Grover problem in adiabatic quantum computation [12] and introduce that it can be solved by order \sqrt{M} .

First of all, we associate M items with M orthonormal bases $|0\rangle, |1\rangle, \dots, |M-1\rangle$. Our purpose is to find $|0\rangle$ corresponding to the target item. We define the target Hamiltonian \hat{H}_P as

$$\hat{H}_P = \hat{I}_M - |0\rangle\langle 0|, \quad (2.21)$$

where \hat{I}_M is the $M \times M$ identity matrix, because the ground state corresponds to the target item. Since there is no information about the target item at the initial time, we also define the driver Hamiltonian \hat{H}_I as

$$\hat{H}_I = \hat{I}_M - |\psi_0\rangle\langle\psi_0|, \quad (2.22)$$

$$|\psi_0\rangle = \frac{1}{\sqrt{M}} \sum_{i=0}^{M-1} |i\rangle\langle i|, \quad (2.23)$$

and the total Hamiltonian $\hat{H}(t)$ is given by

$$\hat{H}(t) = (1 - f(t))\hat{H}_I + f(t)\hat{H}_P, \quad (2.24)$$

where $0 \leq f(t) \leq 1$, $f(0) = 0$ and $f(1) = 1$.

Selecting $|0\rangle$ and

$$|\Psi\rangle = \frac{1}{\sqrt{M-1}} \sum_{i=1}^{M-1} |i\rangle \quad (2.25)$$

$$|\phi_\alpha\rangle = \frac{1}{\sqrt{\alpha(\alpha+1)}} \left[\sum_{i=1}^{\alpha} |i\rangle - \alpha|\alpha+1\rangle \right] \quad (2.26)$$

as the basis, we can rewrite $\hat{H}(t)$ as

$$\hat{H}(t) = \begin{pmatrix} (1-f(t))\left(1-\frac{1}{M}\right) & -(1-f(t))\frac{\sqrt{M-1}}{M} & & \\ -(1-f(t))\frac{\sqrt{M-1}}{M} & (1-f(t))\frac{1}{M} & & \\ & & & \hat{I}_{M-2} \end{pmatrix}. \quad (2.27)$$

When we start from the the trivial ground state of \hat{H}_I , the dynamics by $\hat{H}(t)$ is restricted to the subspace spanned by $|0\rangle$ and $|\Psi\rangle$, which means that, in the process of adiabatic quantum computation, we need only consider this subspace. Then, we immediately find that the ground energy $E_0(t)$ and the first excited energy $E_1(t)$ are given by

$$E_0(t) = \frac{1 - \sqrt{1 - 4\frac{M-1}{M}f(t)(1-f(t))}}{2}, \quad (2.28)$$

$$E_1(t) = \frac{1 + \sqrt{1 - 4\frac{M-1}{M}f(t)(1-f(t))}}{2}, \quad (2.29)$$

$$E_1(t) - E_0(t) = \sqrt{1 - 4\frac{M-1}{M}f(t)(1-f(t))}. \quad (2.30)$$

Because the minimum value of the energy gap is just $\sqrt{1/M}$ at $f(t) = 1/2$, the adiabatic theorem naively suggests that the computational time is $1/\Delta^2 \propto M$ [12], which is the same as the computational complexity of classical algorithms. Against this difficulty, Roland and Cerf [57] proposed the local adiabatic quantum evolution in which the Hamiltonian slowly changes in the region where the energy gap is small and vice versa. Then, they showed that the computational time is reduced to order \sqrt{M} , that is, quantum acceleration is also realized in adiabatic quantum computation.

In the Grover problem, it is shown that the computational time of order \sqrt{M} is optimal in the quantum circuit model [88]. Is order \sqrt{M} is also optimal in quantum annealing? Similar argument is also proposed in Ref. [57], However, the proof of the optimality of order \sqrt{M} is quite complicated and there is a point. Fortunately, recent studies have proved the optimality of order \sqrt{M} by using the quantum speed limit [40, 41]. This will be discussed in detail in the next section.

Finally, after describing the relation between the p -spin model and the Grover problem, we end this section. When we assume p to be odd and take the limit of $p \rightarrow \infty$ in the p -spin model,

$$\hat{H} = -N \left(\frac{1}{N} \sum_{i=1}^N \hat{\sigma}_i^z \right)^p, \quad (2.31)$$

the eigenenergy of \hat{H} is 1 only for $\hat{m}_z = 1$ and otherwise 0 for $\hat{m}_z \neq 1$. This energy structure is the same as the Grover problem, which means that the Grover problem is equivalent to the problem of finding the ground state of the p -spin model in $p \rightarrow \infty$. We note that $M = 2^N$, where M is the number of items and N is the number of spins. In addition, in the limit of $p \rightarrow \infty$, the XX interaction can not avoid the first order phase transition [23], which is consistent with the optimality of the Grover problem.

2.4. Quantum speed limit and Grover problem

Until now, we have discussed static problems with adiabatic quantum computation in mind because static problems are easier to analyze than dynamical problems. Then, is it possible to investigate the limitations of the performance of adiabatic quantum computation from the viewpoint of dynamics? The quantum speed limit [38,39] gives an upper limit to the time evolution of quantum systems and limits quantum dynamics. In this section, we introduce the quantum speed limit. Firstly, we explain the Mandelstam–Tamm bound [38] as the representative work. Next, we introduce another quantum speed limit which is called the Kieu bound [89]. As an application for adiabatic quantum computation, recent studies [40,41] showed that, using the Kieu bound, the optimal computational time of the Grover problem is also of order \sqrt{M} for the problem size M in adiabatic quantum computation. Finally, we discuss what the quantum speed limit will be in classical systems.

2.4.1. Quantum speed limit

We consider the time-independent Hamiltonian \hat{H} . The state $|\phi(t)\rangle$ of the system satisfies the Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t} |\phi(t)\rangle = \hat{H} |\phi(t)\rangle. \quad (2.32)$$

Then, the minimal evolution time τ_{QSL} needed for the state to rotate orthogonally is bounded as [38],

$$\tau \geq \tau_{\text{QSL}} = \frac{\pi\hbar}{2\Delta E}, \quad (2.33)$$

where ΔE is the energy variance defined as $\sqrt{\langle\phi|\hat{H}^2|\phi\rangle - \langle\phi|\hat{H}|\phi\rangle^2}$. This inequality is known as the Mandelstam–Tamm bound [38]. This result implied that quantum mechanics has a fundamental speed limit characterized by Planck’s constant, and thus, the above inequality is called the energy-time uncertainty relation or quantum speed limit (QSL). The quantum speed limit can be also regarded as a trade-off between energy and time in the variance of a state.

The above results are extended to time-dependent systems and two states not orthogonal to each other, and it is known that the following inequality holds for general time-dependent systems [97, 101]

$$\tau \geq \frac{\arccos(|\langle\phi(t)|\phi(0)\rangle|)}{\frac{1}{\tau} \int_0^\tau dt \Delta E(t)}, \quad (2.34)$$

where $\Delta E(t)$ is defined as $\sqrt{\langle\phi(t)|\hat{H}^2(t)|\phi(t)\rangle - \langle\phi(t)|\hat{H}(t)|\phi(t)\rangle^2}$. The result of QSL is geometrically clear and it means that, when the distance between two states is defined properly, the time evolution along the geodesic line is the shortest path. Investigating the restrictions on the time evolution of quantum dynamics is an interesting and important problem, and there are many related works: an alternative quantum speed limit [39], the shortest time for quantum computation [90], cases on mixed states [91], time-dependent systems [45, 92, 93], and open systems [94–96], geometric derivations of the QSL [97–101], and various applications [102–109].

2.4.2. Another type of quantum speed limit for Grover problem

Although the results of QSL are mathematically elegant, it is, in general, very difficult to evaluate the bound for a given time-dependent Hamiltonian and initial state because it requires information on the intermediate state of time evolution. On the other hand, there is another class of QSL and it is not only formal but also suitable for actually evaluating the speed limit [41, 89, 93]. For example, for a given Hamiltonian $\hat{H}(t)$, the initial state $|\psi_0\rangle$ and the state $|\psi(\tau)\rangle$ following the Schrödinger equation, Kieu [89] derived the following inequality

$$\hbar\| |\psi(\tau)\rangle - e^{-i \int_0^\tau ds \alpha(s)} |\psi_0\rangle \| \leq \int_0^\tau dt \| (\hat{H}(t) - \alpha(t)) |\psi_0\rangle \|, \quad (2.35)$$

where $\alpha(t)$ is an arbitrary time-dependent function. Note that Eq. (2.35) contains only the initial state and the given Hamiltonian, and does not require the information on the intermediate state of the dynamics. This enables us to easily evaluate the right hand side of Eq. (2.35). In addition, Eq. (2.35) is not only computable but also tight. Recent study [40,41] shows that, using Eq. (2.35), the following relation holds,

$$\tau \geq \sqrt{2M}, \quad (2.36)$$

where τ is the minimum required time to reach the target state from the initial state in the Grover problem. This means that the optimal computational time of the Grover problem is of order \sqrt{M} in quantum annealing. Therefore, the quantum speed limit is also very useful for quantum annealing, and there exists a limit to the speed of the computational time of quantum annealing in general. As a matter of course, it is impossible to infinitely shorten the calculation time of quantum annealing.

2.4.3. Quantum speed limit in the classical limit

The quantum speed limit was originally discovered from the motivation to explore the uncertainty principle between time and energy and has been unique in quantum mechanics. Recent studies [42–45] argued that the quantum speed limit vanishes in the classical limit. For this reason, does the counterpart of the quantum speed limit not exist in classical systems? In addition, if the quantum speed limit is characteristic of quantum systems, does it mean that simulated annealing, which is a classical algorithm corresponding quantum annealing, has no limitation of time evolution?

In Sec. 4, we answer these questions. We clarify that the quantum speed limit is not a phenomenon particular to quantum systems and the dynamics of the classical Liouville equation is also restricted by the "classical speed limit" which corresponds to the quantum speed limit. Furthermore, we obtain similar speed limits for the imaginary-time Schrödinger equation such as the classical master equation. This result means that there is an upper bound of time evolution for simulated annealing, which is a natural result.

3. Exact partition functions for mean-field quantum spin systems

As we pointed out in the previous chapter, mean-field quantum spin systems have not been solved without static approximation, and its exactness has not been proven even for models where the static approximation seems to be exact. The purpose of this chapter is to clarify when the static approximation is exact and solve mean-field quantum spin systems exactly. In order to deal with the imaginary-time dependence of the partition function exactly, we use the optimal control theory [46, 47]. The optimal control theory is originally developed in the field of control engineering and is a theory of determining the time dependence of the coefficients of the differential equations so as to minimize (or maximize) a given cost function. Then, we have to solve the corresponding classical Hamilton's equations for special initial and terminal conditions. Identifying the problem of determining the imaginary-time dependence of the partition function as the optimal control problem in the imaginary-time Schrödinger equation, we obtain the partition function of a wider class of mean-field quantum spin systems exactly.

First, we demonstrate our method for the simplest mean-field quantum spin system, the p -spin model with transverse field, in Sec. 3.1. We show that the static approximation gives the exact solution for the p -spin model with transverse field in the thermodynamic limit. Section 3.2 generalizes our method to the generalized Hopfield model with finite-number patterns. In Sec. 3.3, as a demonstration, we show that the previous studies, treated in Sec. 2.2.1, 2.2.2 and 2.2.3, are exact where the non-stoquastic Hamiltonian and the inhomogeneous transverse field accelerate the computational time exponentially for mean-field quantum spin systems. Furthermore, Sec. 3.4 is devoted to a further generalization of Sec. 3.2. We prove that the static approximation is also exact for a wider class of mean-field quantum spin systems in general. In Sec. 3.5, we prove that the nonlinear classical Hamiltonian, which appeared in the process of solv-

ing the optimal control problem, belongs to integrable system in the sense of the Liouville integrability. In other words, the nonlinear classical Hamilton systems treated in this chapter are just classical nonlinear integrable systems. To the best of our knowledge, our nonlinear classical integrable systems have been not been known so far. Finally, in Sec. 3.6, we give summary and discussion. We also note that our method can not be applied to the Hopfield model with infinite-number patterns and the p -spin-interacting spin glass model in the transverse field.

This chapter is based on my work in Ref. [110].

3.1. p -spin model with transverse field

First, as a simple case, we consider the infinite-range ferromagnetic p -spin model with the transverse field term,

$$\begin{aligned}\hat{H} &= -\frac{1}{N^{p-1}} \left(\sum_{i=1}^N \hat{\sigma}_i^z \right)^p - \Gamma \sum_{i=1}^N \hat{\sigma}_i^x \\ &= \hat{H}_0 + \hat{V},\end{aligned}\tag{3.1}$$

where we define $\hat{H}_0 = -\frac{1}{N^{p-1}} \left(\sum_{i=1}^N \hat{\sigma}_i^z \right)^p$ and $\hat{V} = -\Gamma \sum_{i=1}^N \hat{\sigma}_i^x$. In this model, it is believed that the static approximation gives the exact solution. In the following, we prove it.

First, we derive the partition function with the imaginary-time dependence. We apply the static approximation and obtain the free energy and the self-consistent equation. We also briefly review the previous studies on the exactness of the static approximation. Next, we translate the problem obtaining the partition function in the thermodynamic limit to the optimal control problem in the imaginary-time Schrödinger equation. Finally, we solve it exactly using the optimal control theory. Although the p -spin model with the transverse field is the simplest mean-field quantum model, all the essence of our method is included in Sec. 3.1.

3.1.1. Derivation of partition function

Following the standard procedure, we will obtain the partition function,

$$\begin{aligned}Z &= \text{Tr} e^{-\beta \hat{H}_0 - \beta \hat{V}} \\ &= \sum_{\{\sigma_i^z = \pm 1\}} \langle \{\sigma_i^z\} | e^{-\beta \hat{H}_0 - \beta \hat{V}} | \{\sigma_i^z\} \rangle\end{aligned}\tag{3.2}$$

where $\{\sigma_i^z = \pm 1\}$ represents the sum on the z bases for all spins and $|\{\sigma_i^z\}\rangle$ describes the orthonormal basis that diagonalizes the z -component of the Pauli matrices. Using the Suzuki-Trotter decomposition,

$$e^{\hat{A}+\hat{B}} = \lim_{M \rightarrow \infty} \left(e^{\hat{A}/M} e^{\hat{B}/M} \right)^M, \quad (3.3)$$

we rewrite the partition function as

$$Z = \lim_{M \rightarrow \infty} \sum_{\{\sigma_i^z = \pm 1\}} \langle \{\sigma_i^z\} | \left(e^{-\beta \hat{H}_0/M} e^{-\beta \hat{V}/M} \right)^M | \{\sigma_i^z\} \rangle. \quad (3.4)$$

Inserting the closure relation

$$\hat{1} = \sum_{\{\sigma_i^z(t) = \pm 1\}} |\{\sigma_i^z(t)\}\rangle \langle \{\sigma_i^z(t)\}| \quad (3.5)$$

into $e^{\hat{A}/M} e^{\hat{B}/M}$, M times, we obtain

$$Z = \lim_{M \rightarrow \infty} \prod_{t=1}^M \sum_{\{\sigma_i^z(t) = \pm 1\}} \langle \{\sigma_i^z(t)\} | e^{-\beta \hat{H}_0/M} e^{-\beta \hat{V}/M} | \{\sigma_i^z(t+1)\} \rangle, \quad (3.6)$$

where $t = 1, 2, \dots, M$ is index of the M closure relations and $\sigma_i^z(t)$ satisfies periodic boundary condition $\sigma_i^z(M+1) = \sigma_i^z(1)$. Since the diagonal elements are c numbers, we can separate the operators as follows,

$$\begin{aligned} Z &= \lim_{M \rightarrow \infty} \prod_{t=1}^M \sum_{\{\sigma_i^z(t) = \pm 1\}} \langle \{\sigma_i^z(t)\} | e^{-\beta H_0(t)/M} e^{-\beta \hat{V}/M} | \{\sigma_i^z(t+1)\} \rangle \\ &= \lim_{M \rightarrow \infty} \prod_{t=1}^M \sum_{\{\sigma_i^z(t) = \pm 1\}} e^{-\beta H_0(t)/M} \langle \{\sigma_i^z(t)\} | e^{-\beta \hat{V}/M} | \{\sigma_i^z(t+1)\} \rangle, \end{aligned} \quad (3.7)$$

where

$$H_0(t) = -N \left(\frac{1}{N} \sum_{i=1}^N \sigma_i^z(t) \right)^p. \quad (3.8)$$

Using the Dirac delta function and its Fourier representation, we can represent $e^{-\beta H_0(t)/M}$ as

$$e^{-\beta H_0(t)/M} = \int dm^z(t) \int d\tilde{m}^z(t) e^{\beta N(m^z(t))^p/M} e^{-N\tilde{m}^z(t)(m^z(t) - \frac{1}{N} \sum_{i=1}^N \sigma_i^z(t))}. \quad (3.9)$$

In addition, since the transverse field term does not depend on the site index i , we find

$$\langle \{\sigma_i^z(t)\} | e^{-\beta \hat{V}/M} | \{\sigma_i^z(t+1)\} \rangle = \prod_{i=1}^N \langle \sigma_i^z(t) | e^{\beta \Gamma \hat{\sigma}_i^z/M} | \sigma_i^z(t+1) \rangle. \quad (3.10)$$

From Eqs. (3.9) and (3.10), we obtain

$$Z = \lim_{M \rightarrow \infty} \prod_{t=1}^M \int_{-1}^1 dm^z(t) \int d\tilde{m}^z(t) e^{\beta N(m^z(t))^p/M} e^{-N\tilde{m}^z(t)m^z(t)} \sum_{\{\sigma_i^z(t)=\pm 1\}} \prod_{i=1}^N \langle \sigma_i^z(t) | e^{\tilde{m}^z(t)\hat{\sigma}_i^z(t)} e^{\beta\Gamma\hat{\sigma}_i^z/M} | \sigma_i^z(t+1) \rangle. \quad (3.11)$$

Furthermore, $\langle \sigma_i^z(t) | e^{\tilde{m}^z(t)\hat{\sigma}_i^z(t)} e^{\beta\Gamma\hat{\sigma}_i^z/M} | \sigma_i^z(t+1) \rangle$ is independent of the site index i which leads to

$$Z = \lim_{M \rightarrow \infty} \prod_{t=1}^M \int_{-1}^1 dm^z(t) \int d\tilde{m}^z(t) e^{\beta N(m^z(t))^p/M} e^{-N\tilde{m}^z(t)m^z(t)} \left(\sum_{\{\sigma^z(t)=\pm 1\}} \langle \sigma^z(t) | e^{\tilde{m}^z(t)\hat{\sigma}^z(t)} e^{\beta\Gamma\hat{\sigma}^z/M} | \sigma^z(t+1) \rangle \right)^N. \quad (3.12)$$

Using the saddle point method for $m^z(t)$, we obtain

$$\tilde{m}^z(t) = \frac{\beta p(m^z(t))^{p-1}}{M}. \quad (3.13)$$

Finally, using the closure relation, the partition function is given by

$$Z = \lim_{M \rightarrow \infty} \left(\prod_{t=1}^M \int_{-1}^1 dm^z(t) \right) e^{-N(p-1)\frac{\beta}{M} \sum_{t=1}^M (m^z(t))^p} \left\{ \text{Tr} \left(\prod_{t=1}^M e^{\frac{\beta}{M} p(m^z(t))^{p-1} \hat{\sigma}^z} e^{\frac{\beta}{M} \Gamma \hat{\sigma}^x} \right) \right\}^N. \quad (3.14)$$

3.1.2. Static approximation

Since the trace of the partition function contains the imaginary-time dependence, it is difficult to proceed for further calculations without some approximations. When we use the static approximation which neglects all the t dependence of the parameter,

$$m^z(t) = m^z = \text{const.}, \quad (3.15)$$

we can take the trace in Eq. (3.14) using the inverse operation of the Trotter decomposition $\lim_{M \rightarrow \infty} \left(e^{\hat{A}/M} e^{\hat{B}/M} \right)^M = e^{\hat{A}+\hat{B}}$,

$$\begin{aligned} \lim_{M \rightarrow \infty} \text{Tr} \left(\prod_{t=1}^M e^{\frac{\beta}{M} p(m^z)^{p-1} \hat{\sigma}^z} e^{\frac{\beta}{M} \Gamma \hat{\sigma}^x} \right) &= \lim_{M \rightarrow \infty} \text{Tr} \left(e^{\frac{\beta}{M} p(m^z)^{p-1} \hat{\sigma}^z} e^{\frac{\beta}{M} \Gamma \hat{\sigma}^x} \right)^M \\ &= \text{Tr} \left(\exp \left[\beta p(m^z)^{p-1} \hat{\sigma}^z + \beta \Gamma \hat{\sigma}^x \right] \right) \\ &= 2 \cosh \left(\beta \sqrt{p^2 (m^z)^{2p-2} + \Gamma^2} \right). \end{aligned} \quad (3.16)$$

Then, we obtain the free energy and the saddle point equation,

$$Z_{\text{SA}} = \int \mathcal{D}m^z e^{-N(p-1)\beta(m^z)^p} \times \left(2 \cosh \left(\beta \sqrt{p^2(m^z)^{2p-2} + \Gamma^2} \right) \right)^N, \quad (3.17)$$

$$\begin{aligned} f_{\text{SA}} &\equiv - \lim_{N \rightarrow \infty} \frac{\log Z_{\text{SA}}}{\beta N} \\ &= (p-1)(m^z)^p - \frac{1}{\beta} \log \left\{ 2 \cosh \left(\beta \sqrt{p^2(m^z)^{2p-2} + \Gamma^2} \right) \right\}, \end{aligned} \quad (3.18)$$

$$m^z = p(m^z)^{p-1} \frac{\tanh \left(\beta \sqrt{p^2(m^z)^{2p-2} + \Gamma^2} \right)}{\sqrt{p^2(m^z)^{2p-2} + \Gamma^2}}, \quad (3.19)$$

which is the standard result for a mean-field quantum spin system.

In general, there is no guarantee that the static approximation is exact, and the following relation holds between the exact solution f and the static approximate solution f_{SA} in the thermodynamic limit,

$$f \leq f_{\text{SA}}. \quad (3.20)$$

However, previous studies [22, 23, 25, 26, 29] implied that the static approximation gives the exact partition function for the p -spin model with the transverse field

$$f = f_{\text{SA}}. \quad (3.21)$$

For example, there is an analytical study [26] based on the classical approximation which supports the result of the static approximation. Using the total spin operator

$$\hat{m}^z = \frac{1}{N} \sum_{i=1}^N \hat{\sigma}_i^z, \quad (3.22)$$

$$\hat{m}^x = \frac{1}{N} \sum_{i=1}^N \hat{\sigma}_i^x, \quad (3.23)$$

we rewrite the Hamiltonian as

$$\hat{H} = -N(\hat{m}^z)^p - \Gamma N \hat{m}^x, \quad (3.24)$$

where \hat{m}^z and \hat{m}^x satisfy

$$[\hat{m}^z, \hat{m}^z] = \frac{1}{N^2} \sum_{i=1}^N (-2i \hat{\sigma}_i^y) = -\frac{2i}{N} \hat{m}^y. \quad (3.25)$$

Then, in the thermodynamic limit $N \rightarrow \infty$, it is expected that the noncommutability of \hat{m}^z and \hat{m}^x can be neglected and we can regard \hat{m}^z and \hat{m}^x as

classical numbers m_z and m_x . Furthermore, in the context of quantum annealing, we start from the eigenstate of \hat{m}_x with the maximum eigenvalue 1 and the Hamiltonian \hat{H} commutes with the total spin operator,

$$\hat{S} = \frac{N}{2} (\hat{m}^x, \hat{m}^y, \hat{m}^z). \quad (3.26)$$

Therefore, the following relation always holds,

$$(\hat{m}^x)^2 + (\hat{m}^y)^2 = 1. \quad (3.27)$$

Then, we can rewrite the classical numbers m_z and m_x as

$$m^z = \sin \theta \quad (3.28)$$

$$m^x = \cos \theta \quad (3.29)$$

$$(m^z)^2 + (m^x)^2 = 1 \quad (3.30)$$

Consequently, it is expected that the ground energy in the thermodynamic limit can be obtained by minimizing the following classical energy

$$E = -(\sin \theta)^p - \Gamma \cos \theta. \quad (3.31)$$

Reference [26] shows that the result of the classical approximation is consistent with the result of the static approximation.

Since the above analysis is completely discussed by classical variables and neglects quantum fluctuations, one may doubt the above result. To investigate quantum effects, Ref. [26] also incorporated the effect of quantum fluctuation based on the Holstein-Primakoff transformation which translates the quantum spin system to a boson system,

$$\hat{S}_z = \frac{N}{2} - \hat{a}^\dagger \hat{a}, \quad (3.32)$$

$$\hat{S}_+ = (N - \hat{a}^\dagger \hat{a})^{1/2} \hat{a}. \quad (3.33)$$

where \hat{a} is a boson operator satisfying $[\hat{a}, \hat{a}^\dagger] = 1$. In the thermodynamic limit, it is possible to calculate the parameter value where the energy gap approaches 0 while taking quantum fluctuation into account, which is also consistent with the analysis based on the static approximation.

In addition, the result of numerical diagonalization up to $N = 140$ spins [23] also shows that the point where the energy gap approaches to 0 coincides with the phase transition point based on the static approximation, which confirms the result of the static approximation.

From the above results, it is believed that the static approximation is exact for the p -spin model with the transverse field. However, these results do not prove the exactness of static approximation. In addition, these analyzes are effective only for systems with uniform interaction, and can not be applied to, for example, the Hopfield model with finite-number patterns.

3.1.3. Mapping to optimal control problem

Our aim is to obtain the exact partition function in the thermodynamic limit. Of course, it is difficult to deal with the trace of Eq. (3.14) directly. Then, we convert the trace of Eq. (3.14) into the imaginary-time Schrödinger equation [86,87]. We consider the following imaginary-time Schrödinger equation,

$$\frac{d}{ds}|\psi(s)\rangle = \begin{pmatrix} \hat{H}_{IM}(s) & 0 \\ 0 & \hat{H}_{IM}(s) \end{pmatrix} |\psi(s)\rangle, \quad (3.34)$$

$$\hat{H}_{IM}(s) = p(m^z(s))^{p-1}\hat{\sigma}^z + \Gamma\hat{\sigma}^x - (p-1)(m^z(s))^p, \quad (3.35)$$

$$|\psi(s)\rangle = \begin{pmatrix} x_1(s) & x_2(s) & x_3(s) & x_4(s) \end{pmatrix}^T, \quad (3.36)$$

$$|\psi(0)\rangle = \begin{pmatrix} 1 & 0 & 0 & 1 \end{pmatrix}^T, \quad (3.37)$$

where $0 \leq s \leq \beta$. Obviously, $x_1(\beta)$ and $x_4(\beta)$ are given by

$$\begin{aligned} x_1(\beta) &= \begin{pmatrix} 1 & 0 \end{pmatrix} \mathcal{T} \exp \left(\int_0^\beta ds \hat{H}_{IM}(s) \right) \begin{pmatrix} x_1(0) \\ x_2(0) \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 \end{pmatrix} \mathcal{T} \exp \left(\int_0^\beta ds \hat{H}_{IM}(s) \right) \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \end{aligned} \quad (3.38)$$

$$\begin{aligned} x_4(\beta) &= \begin{pmatrix} 0 & 1 \end{pmatrix} \mathcal{T} \exp \left(\int_0^\beta ds \hat{H}_{IM}(s) \right) \begin{pmatrix} x_3(0) \\ x_4(0) \end{pmatrix} \\ &= \begin{pmatrix} 0 & 1 \end{pmatrix} \mathcal{T} \exp \left(\int_0^\beta ds \hat{H}_{IM}(s) \right) \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \end{aligned} \quad (3.39)$$

where \mathcal{T} means the time ordered product. Then, we find that the trace of Eq. (3.14) is equivalent to $x_1(\beta) + x_4(\beta)$,

$$\lim_{M \rightarrow \infty} \prod_{t=1}^M e^{\frac{\beta}{M} p(m^z(t))^{p-1} \hat{\sigma}^z} e^{\frac{\beta}{M} \Gamma \hat{\sigma}^x} e^{-\frac{\beta}{M} (p-1)(m^z(t))^p} = \mathcal{T} \exp \left(\int_0^\beta ds \hat{H}_{IM}(s) \right), \quad (3.40)$$

$$\lim_{M \rightarrow \infty} \text{Tr} \left(\prod_{t=1}^M e^{\frac{\beta}{M} p(m^z(t))^{p-1} \hat{\sigma}^z} e^{\frac{\beta}{M} \Gamma \hat{\sigma}^x} e^{-\frac{\beta}{M} (p-1)(m^z(t))^p} \right) = x_1(\beta) + x_4(\beta). \quad (3.41)$$

So far, the imaginary-time dependence of $m^z(s)$ is arbitrary, and the partition function is calculated by summing up over arbitrary paths. However, in the thermodynamic limit, only the path with the largest value of $x_1(\beta) + x_4(\beta)$ contributes to the partition function. Therefore, if we can find the imaginary-time dependence of $m^z(s)$ such that the value of $x_1(\beta) + x_4(\beta)$ is the largest in Eq. (3.34), the partition function can be exactly obtained in the thermodynamic limit. The problem of finding the time dependence of the coefficients of the differential equation so as to maximize the given cost function is equivalent to the optimal control problem and, in the following, we will find the optimal imaginary-time dependence of $m^z(s)$ using the method of the optimal control theory.

3.1.4. Optimal control theory

In this subsection, we provide some knowledge about the optimal control theory [46, 47].

For m differential equations describing the motion of m dimensional vector $x(s)$,

$$\dot{x}(s) = f(x(s), u(s)), \quad x(0) = x_0, \quad (3.42)$$

let us consider the problem of finding the control input $u(s) \in U(0, T)$ that minimizes the cost function,

$$J = L_f(x(T)) + \int_0^T ds L(x(s), u(s)), \quad (3.43)$$

where the initial state x_0 and the final time T are known and the final state $x(T)$ is arbitrary. Here, using the auxiliary variable k which is the m -dimensional vector, we define the following function,

$$H_{\text{op}} = k^T f(x, u) - L(x, u), \quad (3.44)$$

then, the following result holds.

A necessary condition for the control input $u^*(t)$ and the corresponding trajectory $x^*(t)$ to be optimal is that there exists a function $k^*(t)$ that simultaneously satisfies the following three conditions (see appendix B.1.1 for proof).

(a) $x^*(t)$ and $k^*(t)$ are solutions to the following ordinary differential equations,

$$\dot{x}^*(s) = \frac{\partial H_{\text{op}}}{\partial k}(x^*(s), u^*(s), k^*(s)), \quad (3.45)$$

$$\dot{k}^*(s) = -\frac{\partial H_{\text{op}}}{\partial x}(x^*(s), u^*(s), k^*(s)). \quad (3.46)$$

(b) $k^*(t)$ satisfies the following boundary condition,

$$k^*(T) = \left. \frac{\partial L_f(x, u)}{\partial x} \right|_{x=x^*(T)}. \quad (3.47)$$

(c) For any time $s \in [0, T]$,

$$\frac{\partial H_{\text{op}}(x^*(s), u^*(s), k^*(s))}{\partial u^*(s)} = 0. \quad (3.48)$$

The above conditions seem to be very difficult at first glance. However, when we regard x and k as position and momentum, Eqs. (3.45) and (3.46) are just the Hamilton's equations. That is, solving the optimal control problem is equivalent to solving the corresponding classical Hamilton's equations for special initial and terminal conditions.

3.1.5. Exact solution of infinite-range ferromagnetic p -spin model

Applying the optimal control theory to our problem, we find that the cost function J is given by

$$J = -x_1(\beta) - x_4(\beta), \quad (3.49)$$

and the imaginary-time Schrödinger equation (3.34) just corresponds to Eq. (3.42). Then, a necessary condition for $m^{z^*}(s)$ and $x^*(s)$ to be optimal is given by (see appendix B.1.2 for detail),

$$\dot{x}_i^*(s) = \frac{\partial H_{\text{op}}^*(x^*(s), k^*(s), m^{z^*}(s))}{\partial k_i}, \quad (3.50)$$

$$\dot{k}_i^*(s) = -\frac{\partial H_{\text{op}}^*(x^*(s), k^*(s), m^{z^*}(s))}{\partial x_i}, \quad (3.51)$$

$$x_1(0) = x_4(0) = 1, \quad (3.52)$$

$$x_2(0) = x_3(0) = 0, \quad (3.53)$$

$$k_1(\beta) = k_4(\beta) = -1, \quad (3.54)$$

$$k_2(\beta) = k_3(\beta) = 0, \quad (3.55)$$

$$\frac{\partial H_{\text{op}}^*(x^*(s), k^*(s), m^{z^*}(s))}{\partial m^{z^*}(s)} = 0, \quad (3.56)$$

where the classical Hamiltonian H_{op} is given by

$$\begin{aligned} H_{\text{op}} = & -(p-1)(m^z)^p \sum_{i=1}^4 x_i k_i + p(m^z)^{p-1} \sum_{i=1}^4 (-1)^{i-1} x_i k_i \\ & + \Gamma(x_1 k_2 + x_2 k_1 + x_3 k_4 + x_4 k_3). \end{aligned} \quad (3.57)$$

From Eq. (3.56), we find

$$m^{z^*}(s) = 0, \quad \frac{\sum_{i=1}^4 (-1)^{i-1} x_i^*(s) k_i^*(s)}{\sum_{i=1}^4 x_i^*(s) k_i^*(s)}. \quad (3.58)$$

As we will see later, since the nontrivial solution,

$$m^{z^*}(s) = \sum_{i=1}^4 (-1)^{i-1} x_i^*(s) k_i^*(s) / \sum_{i=1}^4 x_i^*(s) k_i^*(s), \quad (3.59)$$

contains the trivial solution $m^{z^*}(s) = 0$, we focus only on the nontrivial solution. Then, although Eq. (3.58) is the necessary condition for $m^{z^*}(s)$, there is only one condition in Eq. (3.58). Thus, if we find one solution, it is just the optimal solution from uniqueness of the optimal control. Equation (3.57) is reduced to

$$H_{\text{op}}^* = \Gamma(x_1 k_2 + x_2 k_1 + x_3 k_4 + x_4 k_3) + \left(\frac{\sum_{i=1}^4 (-1)^{i-1} x_i k_i}{\sum_{i=1}^4 x_i k_i} \right)^p \sum_{i=1}^4 x_i k_i. \quad (3.60)$$

Obviously, it is difficult to find a general solution of the Hamilton equations of H_{op}^* except for $p = 1$. However, we will see that the solution of H_{op}^* can be just obtained in the case where the boundary conditions are given by Eqs. (3.52)-(3.55).

From the Hamilton equations of H_{op}^* , the equation of motion of $m^{z^*}(s)$ is given by

$$\frac{d}{ds} m^{z^*}(s) = - \frac{2\Gamma(x_1^* k_2^* - x_2^* k_1^* + x_3^* k_4^* - x_4^* k_3^*)}{x_1^* k_1^* + x_2^* k_2^* + x_3^* k_3^* + x_4^* k_4^*}. \quad (3.61)$$

Here, we consider the Hamilton equations of H_{op} when m^z is constant. We

immediately find the solutions of $x_i^C(s)$ and $k_i^C(s)$ as follows,

$$\begin{aligned} \begin{pmatrix} x_1^C(s) \\ x_2^C(s) \\ x_3^C(s) \\ x_4^C(s) \end{pmatrix} &= \begin{pmatrix} e^{s\{p(m^z)^{p-1}\hat{\sigma}^z + \Gamma\hat{\sigma}^x - (p-1)(m^z)^p\}} & 0 \\ 0 & e^{s\{p(m^z)^{p-1}\hat{\sigma}^z + \Gamma\hat{\sigma}^x - (p-1)(m^z)^p\}} \end{pmatrix} \begin{pmatrix} x_1(0) \\ x_2(0) \\ x_3(0) \\ x_4(0) \end{pmatrix} \\ &= e^{-s(p-1)(m^z)^p} \begin{pmatrix} \cosh\left(s\sqrt{p^2(m^z)^{2p-2} + \Gamma^2}\right) + \frac{p(m^z)^{p-1} \sinh\left(s\sqrt{p^2(m^z)^{2p-2} + \Gamma^2}\right)}{\sqrt{p^2(m^z)^{2p-2} + \Gamma^2}} \\ \frac{\Gamma \sinh\left(s\sqrt{p^2(m^z)^{2p-2} + \Gamma^2}\right)}{\sqrt{p^2(m^z)^{2p-2} + \Gamma^2}} \\ \frac{\Gamma \sinh\left(s\sqrt{p^2(m^z)^{2p-2} + \Gamma^2}\right)}{\sqrt{p^2(m^z)^{2p-2} + \Gamma^2}} \\ \cosh\left(s\sqrt{p^2(m^z)^{2p-2} + \Gamma^2}\right) - \frac{p(m^z)^{p-1} \sinh\left(s\sqrt{p^2(m^z)^{2p-2} + \Gamma^2}\right)}{\sqrt{p^2(m^z)^{2p-2} + \Gamma^2}} \end{pmatrix}, \end{aligned} \quad (3.62)$$

$$\begin{pmatrix} k_1^C(s) \\ k_2^C(s) \\ k_3^C(s) \\ k_4^C(s) \end{pmatrix} = - \begin{pmatrix} x_1^C(\beta - s) \\ x_2^C(\beta - s) \\ x_3^C(\beta - s) \\ x_4^C(\beta - s) \end{pmatrix}. \quad (3.63)$$

Then, we find

$$x_1^C(s)k_2^C(s) - x_2^C(s)k_1^C(s) + x_3^C(s)k_4^C(s) - x_4^C(s)k_3^C(s) = 0. \quad (3.64)$$

Thus, when we put $m^z(s)$ as

$$m^{zC}(s) = \frac{\sum_{i=1}^4 (-1)^{i-1} x_i^C(s) k_i^C(s)}{\sum_{i=1}^4 x_i^C(s) k_i^C(s)}, \quad (3.65)$$

in the Hamilton equations of H_{op} , then we find that $m^{zC}(s)$ is constant

$$\frac{d}{ds} m^{zC}(s) = 0, \quad (3.66)$$

and the solution of H_{op} are also given by $x_i^C(s)$, $k_i^C(s)$ and $m^{zC}(s)$. In addition, we find that this solution is simultaneously the solution of H_{op}^* because Eq. (3.58) is satisfied. Therefore, from uniqueness of the optimal control, this is just the solution of the motion of H_{op}^* , *i.e.*, the solution of the optimal control problem is given by

$$x_i^*(s) = x_i^C(s), \quad (3.67)$$

$$k_i^*(s) = k_i^C(s), \quad (3.68)$$

under the condition of Eq. (3.65). Furthermore, the condition (3.65) reproduces the self-consistent equation of the static approximation (3.19),

$$m^{zC}(\beta) = \frac{x_1^C(\beta) - x_4^C(\beta)}{x_1^C(\beta) + x_4^C(\beta)} = p(m^z)^{p-1} \frac{\tanh\left(\beta\sqrt{p^2(m^{zC})^{2p-2} + \Gamma^2}\right)}{\sqrt{p^2(m^{zC})^{2p-2} + \Gamma^2}}. \quad (3.69)$$

As a result, the optimal solution is equivalent to the static approximate solution and the static approximation is exact for the infinite-range ferromagnetic p -spin model.

3.2. Generalized Hopfield model with finite-number patterns

Although we have considered the simple system so far, a similar analysis is straightforwardly applicable to the generalized Hopfield model,

$$\hat{H}_G = -N \sum_{\mu=1}^k f_{\mu} \left(\frac{1}{N} \sum_{i=1}^N J_i^{\mu} \hat{\sigma}_i^z \right) - N \sum_{\nu=1}^l g_{\nu} \left(\frac{1}{N} \sum_{i=1}^N \Gamma_i^{\nu} \hat{\sigma}_i^x \right), \quad (3.70)$$

where f_{μ} and g_{ν} are arbitrary functions and J_i^{μ} and Γ_i^{ν} depend on site i . Later, we will show that this Hamiltonian contains many mean-field quantum spin systems analyzed in the context of quantum annealing. The partition function is as follows (see appendix C.1 for details)

$$Z = \lim_{M \rightarrow \infty} \left(\prod_{t=1}^M \int dm_{\mu}^z(t) \int dm_{\nu}^x(t) \right) \prod_{i=1}^N \left\{ \text{Tr} \left(\prod_{t=1}^M e^{\frac{\beta}{M} \sum_{\mu} J_i^{\mu} f'_{\mu}(m_{\mu}^z(t)) \hat{\sigma}_i^z} e^{\frac{\beta}{M} \sum_{\nu} \Gamma_i^{\nu} g'_{\nu}(m_{\nu}^x(t)) \hat{\sigma}_i^x} e^{\frac{\beta}{M} \left\{ \sum_{\mu} (-f'_{\mu}(m_{\mu}^z(t)) \cdot m_{\mu}^z(t) + f_{\mu}(m_{\mu}^z(t))) + \sum_{\nu} (-g'_{\nu}(m_{\nu}^x(t)) \cdot m_{\nu}^x(t) + g_{\nu}(m_{\nu}^x(t))) \right\}} \right) \right\}. \quad (3.71)$$

In the following, we will prove that the static approximation is also exact for the generalized Hopfield model.

3.2.1. Mapping to optimal control problem

Firstly, we regard the integrand of the partition function as the result of the imaginary-time Schrödinger equation. We consider the following imaginary-time

Schrödinger equation,

$$\frac{d}{ds}|\psi(s)\rangle = \begin{pmatrix} \hat{H}_{IM,1}(s) & 0 & 0 & 0 \\ 0 & \hat{H}_{IM,2}(s) & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & \hat{H}_{IM,N}(s) \end{pmatrix} |\psi(s)\rangle, \quad (3.72)$$

$$\begin{aligned} \hat{H}_{IM,i}(s) &= \sum_{\mu} J_i^{\mu} f'_{\mu}(m_{\mu}^z(t)) \hat{\sigma}^z + \sum_{\nu} \Gamma_i^{\nu} g'_{\nu}(m_{\nu}^x(t)) \hat{\sigma}^x \\ &+ \sum_{\mu} \left(-f'_{\mu}(m_{\mu}^z(t)) \cdot m_{\mu}^z(t) + f_{\mu}(m_{\mu}^z(t)) \right) \\ &+ \sum_{\nu} \left(-g'_{\nu}(m_{\nu}^x(t)) \cdot m_{\nu}^x(t) + g_{\nu}(m_{\nu}^x(t)) \right), \end{aligned} \quad (3.73)$$

$$|\psi(s)\rangle = \begin{pmatrix} x_1(s) & x_2(s) & x_3(s) & x_4(s) & \cdots & x_{4N-3}(s) & x_{4N-2}(s) & x_{4N-1}(s) & x_{4N}(s) \end{pmatrix}^{\text{T}}, \quad (3.74)$$

$$|\psi(0)\rangle = \begin{pmatrix} 1 & 0 & 0 & 1 & \cdots & 1 & 0 & 0 & 1 & \cdots & 1 & 0 & 0 & 1 \end{pmatrix}^{\text{T}}, \quad (3.75)$$

where $0 \leq s \leq \beta$. From the same discussion as before, we find that, in the thermodynamic limit, the trace of the partition function is evaluated as

$$\begin{aligned} &\lim_{N \rightarrow \infty} \lim_{M \rightarrow \infty} \prod_{i=1}^N \left\{ \text{Tr} \left(\prod_{t=1}^M e^{\frac{\beta}{M} \sum_{\mu} J_i^{\mu} f'_{\mu}(m_{\mu}^z(t)) \hat{\sigma}^z} e^{\frac{\beta}{M} \sum_{\nu} \Gamma_i^{\nu} g'_{\nu}(m_{\nu}^x(t)) \hat{\sigma}^x} \right. \right. \\ &\quad \left. \left. e^{\frac{\beta}{M} \left\{ \sum_{\mu} \left(-f'_{\mu}(m_{\mu}^z(t)) \cdot m_{\mu}^z(t) + f_{\mu}(m_{\mu}^z(t)) \right) + \sum_{\nu} \left(-g'_{\nu}(m_{\nu}^x(t)) \cdot m_{\nu}^x(t) + g_{\nu}(m_{\nu}^x(t)) \right) \right\}} \right) \right\} \\ &= \lim_{N \rightarrow \infty} \prod_{i=1}^N (x_{4i-3}^*(\beta) + x_{4i-3}^*(\beta)), \end{aligned} \quad (3.76)$$

where x_i^* is the optimal solution of the following optimal control problem (see appendix B.1.3 for detail),

$$\dot{x}_i^*(s) = \frac{\partial H_{G,\text{op}}}{\partial k_i}(x^*(s), k^*(s), m_{\mu}^{z*}(s), m_{\nu}^{x*}(s)), \quad (3.77)$$

$$\dot{k}_i^*(s) = -\frac{\partial H_{G,\text{op}}}{\partial x_i}(x^*(s), k^*(s), m_{\mu}^{z*}(s), m_{\nu}^{x*}(s)), \quad (3.78)$$

$$x_{4j-3}(0) = x_{4j}(0) = 1, \quad (3.79)$$

$$x_{4j-2}(0) = x_{4j-1}(0) = 0, \quad (3.80)$$

$$k_{4j-3}(\beta) = k_{4j}(\beta) = -\prod_{i=1, i \neq j}^N (x_{4i-3}(\beta) + x_{4i}(\beta)), \quad (3.81)$$

$$k_{4j-2}(\beta) = k_{4j-1}(\beta) = 0, \quad (3.82)$$

$$\frac{\partial H_{G,\text{op}}^*(x^*(s), k^*(s), m_{\mu}^{z*}(s), m_{\nu}^{x*}(s))}{\partial m_{\mu}^{z*}(s)} = \frac{\partial H_{G,\text{op}}^*(x^*(s), k^*(s), m_{\mu}^{z*}(s), m_{\nu}^{x*}(s))}{\partial m_{\nu}^{x*}(s)} = 0, \quad (3.83)$$

where the classical Hamiltonian $H_{G,op}$ is given by

$$\begin{aligned}
& H_{G,op}(x, k, m_\mu^z, m_\nu^x) \\
&= \left\{ \sum_\mu \left(-f'_\mu(m_\mu^z) m_\mu^z + f_\mu(m_\mu^z) \right) + \sum_\nu \left(-g'_\nu(m_\nu^x) m_\nu^x + g_\nu(m_\nu^x) \right) \right\} \sum_{i=1}^{4N} x_i k_i \\
&+ \sum_\mu \sum_{i=1}^N J_i^\mu f'_\mu(m_\mu^z) (x_{4i-3} k_{4i-3} - x_{4i-2} k_{4i-2} + x_{4i-1} k_{4i-1} - x_{4i} k_{4i}) \\
&+ \sum_\nu \sum_{i=1}^N \Gamma_i^\nu g'_\nu(m_\nu^x) (x_{4i-3} k_{4i-2} + x_{4i-2} k_{4i-3} + x_{4i-1} k_{4i} + x_{4i} k_{4i-1}). \quad (3.84)
\end{aligned}$$

Therefore, finding the exact solution of the partition function is reduced to solving the $4N$ -dimensional classical Hamiltonian.

3.2.2. Exact solution of the generalized Hopfiled model with finite-number patterns

From Eq. (3.83), we find

$$m_\mu^{z*}(s) = \frac{\sum_{i=1}^N J_i^\mu (x_{4i-3}^* k_{4i-3}^* - x_{4i-2}^* k_{4i-2}^* + x_{4i-1}^* k_{4i-1}^* - x_{4i}^* k_{4i}^*)}{\sum_{i=1}^{4N} x_i^* k_i^*}, \quad (3.85)$$

$$m_\nu^{x*}(s) = \frac{\sum_{i=1}^N \Gamma_i^\nu (x_{4i-3}^* k_{4i-2}^* + x_{4i-2}^* k_{4i-3}^* + x_{4i-1}^* k_{4i}^* + x_{4i}^* k_{4i-1}^*)}{\sum_{i=1}^{4N} x_i^* k_i^*}, \quad (3.86)$$

and Eq. (3.83) is reduced to

$$\begin{aligned}
H_{G,op}^* &= \sum_\mu f_\mu \left(\frac{\sum_{i=1}^N J_i^\mu (x_{4i-3} k_{4i-3} - x_{4i-2} k_{4i-2} + x_{4i-1} k_{4i-1} - x_{4i} k_{4i})}{\sum_{i=1}^{4N} x_i k_i} \right) \sum_{i=1}^{4N} x_i k_i \\
&+ \sum_\nu g_\nu \left(\frac{\sum_{i=1}^N \Gamma_i^\nu (x_{4i-3} k_{4i-2} + x_{4i-2} k_{4i-3} + x_{4i-1} k_{4i} + x_{4i} k_{4i-1})}{\sum_{i=1}^{4N} x_i k_i} \right) \sum_{i=1}^{4N} x_i k_i. \quad (3.87)
\end{aligned}$$

Using the Hamilton equations of $H_{G,op}^*$, we find

$$\frac{d}{ds} m_\mu^{z*}(s) = -2 \frac{\sum_\nu \sum_{i=1}^N g_\nu \Gamma_j^\nu (x_{4i-3}^* k_{4i-2}^* - x_{4i-2}^* k_{4i-3}^* + x_{4i-1}^* k_{4i}^* - x_{4i}^* k_{4i-1}^*)}{\sum_{i=1}^{4N} x_i^* k_i^*}, \quad (3.88)$$

$$\frac{d}{ds} m_\nu^{x*}(s) = 2 \frac{\sum_\mu \sum_{i=1}^N f'_\mu J_j^\mu (x_{4i-3}^* k_{4i-2}^* - x_{4i-2}^* k_{4i-3}^* + x_{4i-1}^* k_{4i}^* - x_{4i}^* k_{4i-1}^*)}{\sum_{i=1}^{4N} x_i^* k_i^*}. \quad (3.89)$$

Here, we consider the Hamilton equations of $H_{G, \text{op}}$ when m_μ^z and m_ν^x are constant. We immediately find the solutions of $x_i^C(s)$ and $k_i^C(s)$ for $i = 1, 2, \dots, 4N$ as follows,

$$x_{4i-3}^C(s) = e^{s\left\{\sum_\mu(-f'_\mu(m_\mu^z)m_\mu^z+f_\mu(m_\mu^z))+\sum_\nu(-g'_\nu(m_\nu^x)m_\nu^x+g_\nu(m_\nu^x))\right\}} \times \left\{ \cosh\left(s\sqrt{\left(\sum_\mu J_i^\mu f'_\mu(m_\mu^z)\right)^2+\left(\sum_\nu \Gamma_i^\nu g'_\nu(m_\nu^x)\right)^2}\right) + \frac{\left(\sum_\mu J_i^\mu f'_\mu(m_\mu^z)\right) \sinh\left(s\sqrt{\left(\sum_\mu J_i^\mu f'_\mu(m_\mu^z)\right)^2+\left(\sum_\nu \Gamma_i^\nu g'_\nu(m_\nu^x)\right)^2}\right)}{\sqrt{\left(\sum_\mu J_i^\mu f'_\mu(m_\mu^z)\right)^2+\left(\sum_\nu \Gamma_i^\nu g'_\nu(m_\nu^x)\right)^2}} \right\}, \quad (3.90)$$

$$x_{4i-2}^C(s) = e^{s\left\{\sum_\mu(-f'_\mu(m_\mu^z)m_\mu^z+f_\mu(m_\mu^z))+\sum_\nu(-g'_\nu(m_\nu^x)m_\nu^x+g_\nu(m_\nu^x))\right\}} \frac{\left(\sum_\nu \Gamma_i^\nu g'_\nu(m_\nu^x)\right) \sinh\left(s\sqrt{\left(\sum_\mu J_i^\mu f'_\mu(m_\mu^z)\right)^2+\left(\sum_\nu \Gamma_i^\nu g'_\nu(m_\nu^x)\right)^2}\right)}{\sqrt{\left(\sum_\mu J_i^\mu f'_\mu(m_\mu^z)\right)^2+\left(\sum_\nu \Gamma_i^\nu g'_\nu(m_\nu^x)\right)^2}}, \quad (3.91)$$

$$x_{4i-1}^C(s) = x_{4i-2}^C(s), \quad (3.92)$$

$$x_{4i}^C(s) = e^{s\left\{\sum_\mu(-f'_\mu(m_\mu^z)m_\mu^z+f_\mu(m_\mu^z))+\sum_\nu(-g'_\nu(m_\nu^x)m_\nu^x+g_\nu(m_\nu^x))\right\}} \times \left\{ \cosh\left(s\sqrt{\left(\sum_\mu J_i^\mu f'_\mu(m_\mu^z)\right)^2+\left(\sum_\nu \Gamma_i^\nu g'_\nu(m_\nu^x)\right)^2}\right) - \frac{\left(\sum_\mu J_i^\mu f'_\mu(m_\mu^z)\right) \sinh\left(s\sqrt{\left(\sum_\mu J_i^\mu f'_\mu(m_\mu^z)\right)^2+\left(\sum_\nu \Gamma_i^\nu g'_\nu(m_\nu^x)\right)^2}\right)}{\sqrt{\left(\sum_\mu J_i^\mu f'_\mu(m_\mu^z)\right)^2+\left(\sum_\nu \Gamma_i^\nu g'_\nu(m_\nu^x)\right)^2}} \right\}, \quad (3.93)$$

$$k_{4i-3}^C(s) = -x_{4i-3}^C(\beta-s) \prod_{i=1, i \neq j}^N (x_{4i-3}(\beta) + x_{4i}(\beta)), \quad (3.94)$$

$$k_{4i-2}^C(s) = -x_{4i-2}^C(\beta-s) \prod_{i=1, i \neq j}^N (x_{4i-3}(\beta) + x_{4i}(\beta)), \quad (3.95)$$

$$k_{4i-1}^C(s) = k_{4i-2}^C(s), \quad (3.96)$$

$$k_{4i}^C(s) = -x_{4i}^C(\beta-s) \prod_{i=1, i \neq j}^N (x_{4i-3}(\beta) + x_{4i}(\beta)). \quad (3.97)$$

Then, we find

$$x_{4i-3}^C(s)k_{4i-2}^C(s) - x_{4i-2}^C(s)k_{4i-3}^C(s) + x_{4i-1}^C(s)k_{4i}^C(s) - x_{4i}^C(s)k_{4i-1}^C(s) = 0. \quad (3.98)$$

Thus, when we put $m_\mu^z(s)$ and $m_\nu^x(s)$ as

$$m_\mu^{zC}(s) = \frac{\sum_{i=1}^N J_i^\mu (x_{4i-3}^C k_{4i-3}^C - x_{4i-2}^C k_{4i-2}^C + x_{4i-1}^C k_{4i-1}^C - x_{4i}^C k_{4i}^C)}{\sum_{i=1}^{4N} x_i^C k_i^C}, \quad (3.99)$$

$$m_\nu^{xC}(s) = \frac{\sum_{i=1}^N \Gamma_i^\nu (x_{4i-3}^C k_{4i-2}^C + x_{4i-2}^C k_{4i-3}^C + x_{4i-1}^C k_{4i}^C + x_{4i}^C k_{4i-1}^C)}{\sum_{i=1}^{4N} x_i^C k_i^C}, \quad (3.100)$$

in the Hamilton equations of $H_{G, \text{op}}$, then we find that $m_\mu^{zC}(s)$ and $m_\nu^{xC}(s)$ are constant

$$\frac{d}{ds} m_\mu^{zC}(s) = 0, \quad (3.101)$$

$$\frac{d}{ds} m_\nu^{xC}(s) = 0, \quad (3.102)$$

and the solution of $H_{G, \text{op}}$ are also given by $x_i^C(s)$, $k_i^C(s)$, $m_\mu^{zC}(s)$, and $m_\nu^{xC}(s)$. In addition, we find that this solution is simultaneously the solution of $H_{G, \text{op}}^*$ because Eq. (3.83) is satisfied. Therefore, from uniqueness of the optimal control, this is just the solution of the motion of $H_{G, \text{op}}^*$, *i.e.*, the solution of the optimal control problem is given by

$$x_i^*(s) = x_i^C(s), \quad (3.103)$$

$$k_i^*(s) = k_i^C(s), \quad (3.104)$$

under the condition of Eq. (3.85). Furthermore, the condition (3.85) and (3.86) reproduce the saddle point equations of the static approximation,

$$\begin{aligned} m_\mu^z &= m_\mu^z(\beta) = \frac{\sum_{i=1}^N J_i^\mu (x_{4i-3}(\beta) k_{4i-3}(\beta) - x_{4i}(\beta) k_{4i}(\beta))}{\sum_{i=1}^N (x_{4i-3}(\beta) k_{4i-3}(\beta) + x_{4i}(\beta) k_{4i}(\beta))} \\ &= \frac{-\prod_i (x_{4i-3}(\beta) + x_{4i}(\beta)) \sum_{i=1}^N J_i^\mu \frac{(x_{4i-3}(\beta) - x_{4i}(\beta))}{x_{4i-3}(\beta) + x_{4i}(\beta)}}{-N \prod_i (x_{4i-3}(\beta) + x_{4i}(\beta))} \\ &= \frac{1}{N} \sum_{i=1}^N J_i^\mu \frac{x_{4i-3}(\beta) - x_{4i}(\beta)}{x_{4i-3}(\beta) + x_{4i}(\beta)} \\ &= \frac{1}{N} \sum_{i=1}^N J_i^\mu \frac{\left(\sum_\mu J_i^\mu f'_\mu(m_\mu^z) \right) \tanh \left(\beta \sqrt{(\sum_\mu J_i^\mu f'_\mu(m_\mu^z))^2 + (\sum_\nu \Gamma_i^\nu g'_\nu(m_\nu^x))^2} \right)}{\sqrt{(\sum_\mu J_i^\mu f'_\mu(m_\mu^z))^2 + (\sum_\nu \Gamma_i^\nu g'_\nu(m_\nu^x))^2}}, \end{aligned} \quad (3.105)$$

$$\begin{aligned}
m_\mu^x &= m_\mu^x(\beta) = \frac{\sum_{i=1}^N \Gamma_i^\nu (x_{4i-2}(\beta)k_{4i-3}(\beta) + x_{4i-1}(\beta)k_{4i}(\beta))}{\sum_{i=1}^N (x_{4i-3}(\beta)k_{4i-3}(\beta) + x_{4i}(\beta)k_{4i}(\beta))} \\
&= \frac{-\prod_i (x_{4i-3}(\beta) + x_{4i}(\beta)) \sum_{i=1}^N \Gamma_i^\nu \frac{(x_{4i-2}(\beta) + x_{4i-1}(\beta))}{x_{4i-3}(\beta) + x_{4i}(\beta)}}{-N \prod_i (x_{4i-3}(\beta) + x_{4i}(\beta))} \\
&= \frac{1}{N} \sum_{i=1}^N \Gamma_i^\nu \frac{x_{4i-2}(\beta) + x_{4i-1}(\beta)}{x_{4i-3}(\beta) + x_{4i}(\beta)} \\
&= \frac{1}{N} \sum_{i=1}^N \Gamma_i^\nu \frac{(\sum_\nu \Gamma_i^\nu g'_\nu(m_\nu^x)) \tanh\left(\beta \sqrt{(\sum_\mu J_i^\mu f'_\mu(m_\mu^z))^2 + (\sum_\nu \Gamma_i^\nu g'_\nu(m_\nu^x))^2}\right)}{\sqrt{(\sum_\mu J_i^\mu f'_\mu(m_\mu^z))^2 + (\sum_\nu \Gamma_i^\nu g'_\nu(m_\nu^x))^2}}.
\end{aligned} \tag{3.106}$$

Therefore, the static approximation is exact for the generalized Hopfield model (3.70).

3.3. Application to quantum annealing

We apply our result to previous studies of quantum annealing, where mean-field quantum spin systems are often used to evaluate the performance of quantum annealing as introduced in Sec. 2.2, and our result guarantees their analysis in general. For example, we consider the Hopfield model with finite-number patterns,

$$\hat{H} = -N \sum_{\mu=1}^k \left(\frac{1}{N} \sum_{i=1}^N J_i^\mu \hat{\sigma}_i^z \right)^p - \Gamma_1 \sum_{i=1}^N \hat{\sigma}_i^x + \Gamma_2 N \left(\frac{1}{N} \sum_{i=1}^N \hat{\sigma}_i^x \right)^2 \tag{3.107}$$

where $\Gamma_1, \Gamma_2 \geq 0$, p is an integer denoting the degree of interactions, and k is an integer representing the finite-number embedded pattern and J_i^μ takes ± 1 at random. The antiferromagnetic multiple- X term is called the non-stoquastic interaction and has been attracting a lot of attention in the field of quantum annealing in recent years. In the process of quantum annealing, recent studies [23, 25] show that, although this system undergoes a first-order phase transition in the absence of the antiferromagnetic multiple- X term, there is a path through a second-order phase transition avoiding a first-order phase transition when the antiferromagnetic multiple- X term is applied. This means that the antiferromagnetic multiple- X term improves exponentially the efficiency of quantum annealing compared with the case only by the transverse field. Although the above result is based on the static approximation, the Hamiltonian (3.107) is included in our Hamiltonian (3.70) when we set $f_\mu(x) = x^p$, $l = 2$, $g_1(x) = \Gamma_1 x$,

$g_2(x) = -\Gamma_2 x^2$, $\Gamma_i^1 = 1$ and $\Gamma_i^2 = 1$. Thus, the result of exponential speed up by the non-stoquastic interaction is exact.

Next, we consider the infinite-range ferromagnetic p -spin model with longitudinal random field,

$$\hat{H} = -N \left(\frac{1}{N} \sum_i \hat{\sigma}_i^z \right)^p - \sum_i h_i \hat{\sigma}_i^z - \sum_i \Gamma_i \hat{\sigma}_i^x, \quad (3.108)$$

where h_i follows the Gaussian distribution with an average of 0 or the binary distribution $h_i = \pm h_0$. Based on the static approximation, a recent study [29] shows that the inhomogeneous transverse field Γ_i can avoid a phase transition in the process of quantum annealing, although the homogeneous transverse field can not avoid a first-order phase transition. This means that the inhomogeneous transverse field accelerates the computation time of quantum annealing exponentially. For $k = 2$, $f_1 = x^p$, $f_2 = x$, $J_i^1 = 1$, $J_i^2 = h_i$, $l = 1$, $g_1 = x$ and $\Gamma_i^1 = \Gamma_i$, our model (3.70) includes the above system (3.108) and certifies the analysis based on the static approximation.

3.4. Further generalization

We have shown that the static approximation is exact for the particular class of mean-field quantum spin systems so far. Although this is a first systematic study on the exactness of the static approximation, the class of mean-field quantum spin systems is a relatively simple system and its partition function is reduced to N non-interacting spins in the time-dependent imaginary-time Schrödinger equation by the Suzuki-Trotter deformation. In order to obtain a solution beyond the static approximation, it is important to obtain further understanding of when the static approximation is exact for mean-field quantum spin systems.

In this section, we further generalize the results of the previous section to a wide class of mean-field quantum spin systems,

$$\hat{H} = -N \sum_{\mu} f_{\mu} \left(\frac{1}{N} \hat{H}_{1,\mu}(\{\hat{\sigma}^z\}) \right) - N \sum_{\nu} g_{\nu} \left(\frac{1}{N} \hat{H}_{2,\nu}(\{\hat{\sigma}^x\}) \right), \quad (3.109)$$

where f_{μ} and g_{ν} are arbitrary functions, $\hat{H}_{1,\mu}(\{\hat{\sigma}^z\})$ and $\hat{H}_{2,\nu}(\{\hat{\sigma}^x\})$ are arbitrary Hamiltonians composed of $\{\hat{\sigma}^z\}$ and $\{\hat{\sigma}^x\}$, respectively. In addition, we assume that their eigenvalues are proportional to the system size N in order to satisfy the extensive property. This Hamiltonian is a generalization of the generalized Hopfield model and has complicated internal structure. We emphasize

that $\hat{H}_{1,\mu}(\{\hat{\sigma}^z\})$ and $\hat{H}_{2,\nu}(\{\hat{\sigma}^x\})$ are allowed in an arbitrary form, which means that this is the most generalization as a natural extension.

In the following, under the assumption that the partition function $\text{Tr} e^{-\beta\hat{H}'}$ for the ancillary Hamiltonian, $\hat{H}' = -\sum_{\mu} J_{\mu}\hat{H}_{1,\mu}(\{\hat{\sigma}^z\}) - \sum_{\nu} \Gamma_{\nu}\hat{H}_{2,\nu}(\{\hat{\sigma}^x\})$, can be calculated for any J_{μ} and Γ_{ν} , we prove that the static approximation is exact for \hat{H} in general. Section 3.4.1 is devoted to obtain the partition function under the static approximation. In Sec 3.4.2, we map the problem of finding the exact partition function to the corresponding optimal control problem. Finally, we solve the corresponding optimal control and show that the optimal solution coincides with the static approximate solution in Sec. 3.4.3.

3.4.1. Partition function and the static approximation

Following the standard procedure, the partition function is given by (see appendix C.2 for details)

$$Z = \int \mathcal{D}m_{\mu}^z \mathcal{D}m_{\nu}^x \text{Tr} \left(\prod_{t=1}^M e^{\frac{\beta}{M} \sum_{\mu} f'_{\mu}(m_{\mu}^z(t)) \hat{H}_{1,\mu}(\{\hat{\sigma}^z\})} e^{\frac{\beta}{M} \sum_{\nu} g'_{\nu}(m_{\nu}^x(t)) \hat{H}_{2,\nu}(\{\hat{\sigma}^x\})} e^{\left[\frac{N\beta}{M} \left\{ -\sum_{\mu} f'_{\mu}(m_{\mu}^z(t)) \cdot m_{\mu}^z(t) + \sum_{\mu} f_{\mu}(m_{\mu}^z(t)) - \sum_{\nu} g'_{\nu}(m_{\nu}^x(t)) \cdot m_{\nu}^x(t) + \sum_{\nu} g_{\nu}(m_{\nu}^x(t)) \right\} \right]} \right), \quad (3.110)$$

When we use the static approximation which neglects the time-dependence of $m_{\mu}^z(t)$ and $m_{\nu}^x(t)$, using the inverse operation of the Suzuki-Trotter decomposition, the partition function is reduced to

$$Z_{\text{SA}} = \int \mathcal{D}m^z e^{N\beta \left\{ -\sum_{\mu} f'_{\mu}(m_{\mu}^z) \cdot m_{\mu}^z + \sum_{\mu} f_{\mu}(m_{\mu}^z) - \sum_{\nu} g'_{\nu}(m_{\nu}^x) \cdot m_{\nu}^x + \sum_{\nu} g_{\nu}(m_{\nu}^x) \right\}} \times \left(\text{Tr} e^{\beta \left(\sum_{\mu} f'_{\mu}(m_{\mu}^z) \hat{H}_{1,\mu}(\{\hat{\sigma}^z\}) + \sum_{\nu} g'_{\nu}(m_{\nu}^x) \hat{H}_{2,\nu}(\{\hat{\sigma}^x\}) \right)} \right). \quad (3.111)$$

Therefore, if we calculate the partition function of \hat{H}' for any J_{μ} and Γ_{ν} , we can write down the self consistent equations

$$m_{\mu}^z = \frac{1}{N} \text{Tr} \left(\hat{H}_{1,\mu}(\{\hat{\sigma}^z\}) e^{\beta \left(\sum_{\mu} f'_{\mu}(m_{\mu}^z) \hat{H}_{1,\mu}(\{\hat{\sigma}^z\}) + \sum_{\nu} g'_{\nu}(m_{\nu}^x) \hat{H}_{2,\nu}(\{\hat{\sigma}^x\}) \right)} \right), \quad (3.112)$$

$$m_{\nu}^x = \frac{1}{N} \text{Tr} \left(\hat{H}_{2,\nu}(\{\hat{\sigma}^x\}) e^{\beta \left(\sum_{\mu} f'_{\mu}(m_{\mu}^z) \hat{H}_{1,\mu}(\{\hat{\sigma}^z\}) + \sum_{\nu} g'_{\nu}(m_{\nu}^x) \hat{H}_{2,\nu}(\{\hat{\sigma}^x\}) \right)} \right). \quad (3.113)$$

Of course, it is very difficult to obtain the partition function of \hat{H}' . Here, based on the assumption that it is possible, in the following, we show that the static approximation is exact.

3.4.2. Mapping to optimal control problem

We consider the 4^N -dimensional imaginary-time Schrödinger equation,

$$\begin{aligned}\hat{H}_{IM}(s) &= \sum_{\mu} f'_{\mu}(m_{\mu}^z(t)) \hat{H}_{1,\mu}(\{\hat{\sigma}^z\}) + \sum_{\nu} g'_{\nu}(m_{\nu}^x(t)) \hat{H}_{2,\nu}(\{\hat{\sigma}^x\}) \\ &\quad + N \left\{ - \sum_{\mu} f'_{\mu}(m_{\mu}^z(t)) \cdot m_{\mu}^z(t) + \sum_{\mu} f_{\mu}(m_{\mu}^z(t)) \right\} \\ &\quad + N \left\{ - \sum_{\nu} g'_{\nu}(m_{\nu}^x(t)) \cdot m_{\nu}^x(t) + \sum_{\nu} g_{\nu}(m_{\nu}^x(t)) \right\}\end{aligned}\quad (3.114)$$

$$|\psi(s)\rangle = \left(x_{1,1}(s) \quad x_{2,1}(s) \quad \cdots \quad x_{2^N,1}(s) \quad x_{1,2}(s) \quad x_{2,2}(s) \quad \cdots \quad x_{2^N,2}(s) \quad \cdots \quad x_{2^N,2^N}(s) \right)^T \quad (3.115)$$

$$x_{i,j}(0) = \delta_{i,j} \quad (3.116)$$

$$\frac{d}{ds} |\psi(s)\rangle = \begin{pmatrix} \hat{H}_{IM}(s) & 0 & 0 & 0 \\ 0 & \hat{H}_{IM}(s) & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & \hat{H}_{IM}(s) \end{pmatrix} |\psi(s)\rangle. \quad (3.117)$$

Then, we find that the trace of Eq. (3.110) coincides with $\sum_{i=1}^{2^N} x_{i,i}(\beta)$,

$$\begin{aligned}\lim_{M \rightarrow \infty} \text{Tr} \left(\prod_{t=1}^M e^{\frac{\beta}{M} \sum_{\mu} f'_{\mu}(m_{\mu}^z(t)) \hat{H}_{1,\mu}(\{\hat{\sigma}^z\})} e^{\frac{\beta}{M} \sum_{\nu} g'_{\nu}(m_{\nu}^x(t)) \hat{H}_{2,\nu}(\{\hat{\sigma}^x\})} \right. \\ \left. \times e^{\left[\frac{N\beta}{M} \left\{ - \sum_{\mu} f'_{\mu}(m_{\mu}^z(t)) \cdot m_{\mu}^z(t) + \sum_{\mu} f_{\mu}(m_{\mu}^z(t)) - \sum_{\nu} g'_{\nu}(m_{\nu}^x(t)) \cdot m_{\nu}^x(t) + \sum_{\nu} g_{\nu}(m_{\nu}^x(t)) \right\} \right]} \right) = \sum_{i=1}^{2^N} x_{i,i}(\beta).\end{aligned}\quad (3.118)$$

Here, we represent the matrix elements of $\hat{H}_{IM}(s)$ as

$$(\hat{H}_{IM}(s))_{i,j} = H_{i,j}(s), \quad (3.119)$$

then, the imaginary-time Schrödinger equation can be rewritten as

$$\dot{x}_{i,j} = \sum_l H_{i,l} x_{l,j}. \quad (3.120)$$

Thus, finding the optimal time-dependence of $m_{\mu}^z(s)$ and $m_{\nu}^z(x)$ is to minimize the following cost function

$$- \sum_{i=1}^{2^N} x_{i,i}(\beta), \quad (3.121)$$

for Eq. (3.117). Therefore, the classical Hamiltonian H_{op} is given by

$$\begin{aligned}
H_{\text{op}} &= \sum_{i,j,l} H_{i,l} x_{l,j} k_{i,j} \\
&= \sum_{\mu} f'_{\mu}(m_{\mu}^z(t)) \sum_{i,j} a_{i,i}^{\mu} x_{i,j} k_{i,j} + \sum_{\nu} g'_{\nu}(m_{\nu}^x(t)) \sum_{i,j,l} b_{i,l}^{\nu} x_{l,j} k_{i,j} \\
&\quad + N \left\{ - \sum_{\mu} f'_{\mu}(m_{\mu}^z(t)) \cdot m_{\mu}^z(t) + \sum_{\mu} f_{\mu}(m_{\mu}^z(t)) \right\} \sum_{i,j} x_{i,j} k_{i,j} \\
&\quad + N \left\{ - \sum_{\nu} g'_{\nu}(m_{\nu}^x(t)) \cdot m_{\nu}^x(t) + \sum_{\nu} g_{\nu}(m_{\nu}^x(t)) \right\} \sum_{i,j} x_{i,j} k_{i,j}, \quad (3.122)
\end{aligned}$$

where $a_{i,i}$ and $b_{i,j}$ represent the matrix elements of $\hat{H}_{1,\mu}(\{\hat{\sigma}^z\})$ and $\hat{H}_{2,\nu}(\{\hat{\sigma}^x\})$, respectively. In addition, the boundary conditions are as follows,

$$x_{i,j}(0) = \delta_{i,j}, \quad (3.123)$$

$$k_{i,j}(\beta) = -\delta_{i,j}. \quad (3.124)$$

3.4.3. Optimal solution

From Eq. (3.48), we obtain

$$m_{\mu}^z(s) = \frac{1}{N} \frac{\sum_{i,j} a_{i,i}^{\mu} x_{i,j} k_{i,j}}{\sum_{i,j} x_{i,j} k_{i,j}}, \quad (3.125)$$

$$m_{\nu}^x(s) = \frac{1}{N} \frac{\sum_{i,j,l} b_{i,l}^{\nu} x_{l,j} k_{i,j}}{\sum_{i,j} x_{i,j} k_{i,j}}. \quad (3.126)$$

Then, H_{op}^* is as follows,

$$\begin{aligned}
H_{\text{op}}^* &= N \sum_{\mu} f_{\mu} \left(\frac{1}{N} \frac{\sum_{i,j} a_{i,i}^{\mu} x_{i,j} k_{i,j}}{\sum_{i,j} x_{i,j} k_{i,j}} \right) \sum_{i,j} x_{i,j} k_{i,j} \\
&\quad + N \sum_{\nu} g_{\nu} \left(\frac{1}{N} \frac{\sum_{i,j,l} b_{i,l}^{\nu} x_{l,j} k_{i,j}}{\sum_{i,j} x_{i,j} k_{i,j}} \right) \sum_{i,j} x_{i,j} k_{i,j}. \quad (3.127)
\end{aligned}$$

The Hamilton's equations of H_{op}^* are given by

$$\begin{aligned}
\frac{dx_{i,j}}{dt} &= x_{i,j} \left(N \sum_{\mu} f_{\mu} + N \sum_{\nu} g_{\nu} - N \sum_{\mu} f'_{\mu} m_{\mu}^z - N \sum_{\nu} g'_{\nu} m_{\nu}^x + \sum_{\mu} f'_{\mu} a_{i,i}^{\mu} \right) \\
&\quad + \sum_{\nu} g'_{\nu} \sum_l b_{i,l}^{\nu} x_{l,j}, \quad (3.128)
\end{aligned}$$

$$\begin{aligned}
\frac{dk_{i,j}}{dt} &= -k_{i,j} \left(N \sum_{\mu} f_{\mu} + N \sum_{\nu} g_{\nu} - N \sum_{\mu} f'_{\mu} m_{\mu}^z - N \sum_{\nu} g'_{\nu} m_{\nu}^x + \sum_{\mu} f'_{\mu} a_{i,i}^{\mu} \right) \\
&\quad - \sum_{\nu} g'_{\nu} \sum_l b_{i,l}^{\nu} k_{l,j}, \quad (3.129)
\end{aligned}$$

where we use $b_{i,j} = b_{j,i}$. In the following, we will show that the boundary conditions (3.123) and (3.124) enable us solve the Hamilton's equation of H_{op}^* .

Using the Hamilton's equations, we obtain the following relations,

$$\frac{d}{dt} \sum_{i,j} x_{i,j} k_{i,j} = 0, \quad (3.130)$$

$$\frac{d}{dt} \sum_{i,j} a_{i,i}^\mu x_{i,j} k_{i,j} = \sum_\nu g'_\nu \sum_{i,j,l} a_{i,i}^\mu b_{i,l}^\nu (x_{l,j} k_{i,j} - x_{i,j} k_{l,j}), \quad (3.131)$$

$$\frac{d}{dt} \sum_{i,j,l} b_{i,l}^\nu x_{l,j} k_{i,j} = \sum_\mu f'_\mu \sum_{i,j,l} a_{i,i}^\mu b_{i,l}^\nu (x_{i,j} k_{l,j} - x_{l,j} k_{i,j}), \quad (3.132)$$

which leads to

$$\frac{d}{ds} m_\mu^z(s) = \frac{1}{N} \frac{\sum_\nu g'_\nu \sum_{i,j,l} a_{i,i}^\mu b_{i,l}^\nu (x_{l,j} k_{i,j} - x_{i,j} k_{l,j})}{\sum_{i,j} x_{i,j} k_{i,j}}, \quad (3.133)$$

$$\frac{d}{ds} m_\nu^x(s) = \frac{1}{N} \frac{\sum_\mu f'_\mu \sum_{i,j,l} a_{i,i}^\mu b_{i,l}^\nu (x_{i,j} k_{l,j} - x_{l,j} k_{i,j})}{\sum_{i,j} x_{i,j} k_{i,j}}. \quad (3.134)$$

Here, we consider the Hamilton's equations of H_{op} when $m_\mu^z(s)$ and $m_\nu^x(s)$ are constant. From the boundary conditions (3.123) and (3.124), we find that the solutions of $x_i^C(s)$ and $k_i^C(s)$ are represented by

$$x_{i,j}^C(s) = \left(e^{s\hat{H}_{IM}} \right)_{i,j} \equiv h_{i,j}(s), \quad (3.135)$$

$$k_{i,j}^C(s) = -h_{i,j}(\beta - s). \quad (3.136)$$

Furthermore, the following relations hold,

$$h_{i,j}(\beta) = \sum_k h_{i,k}(s) h_{k,j}(\beta - s) = \sum_k h_{i,k}(\beta - s) h_{k,j}(s), \quad (3.137)$$

$$h_{i,j}(s) = h_{j,i}(s). \quad (3.138)$$

Then, we obtain

$$\begin{aligned} \sum_j (x_{i,j}^C(s) k_{i,j}^C(s) - x_{i,j}^C(s) k_{l,j}^C(s)) &= - \sum_j (h_{l,j}(s) h_{i,j}(\beta - s) - h_{i,j}(s) h_{l,j}(\beta - s)) \\ &= -(h_{l,i}(\beta) - h_{i,l}(\beta)) \\ &= 0. \end{aligned} \quad (3.139)$$

Therefore, when we put $m_\mu^z(s)$ and $m_\nu^x(s)$ as

$$m_\mu^z(s) = \frac{1}{N} \frac{\sum_{i,j} a_{i,i}^\mu x_{i,j}^C(s) k_{i,j}^C(s)}{\sum_{i,j} x_{i,j}^C(s) k_{i,j}^C(s)}, \quad (3.140)$$

$$m_\nu^x(s) = \frac{1}{N} \frac{\sum_{i,j,l} b_{i,l}^\nu x_{l,j}^C(s) k_{i,j}^C(s)}{\sum_{i,j} x_{i,j}^C(s) k_{i,j}^C(s)}, \quad (3.141)$$

in the Hamilton's equations of H_{op} , then we find that $m_{\mu}^{zC}(s)$ and $m_{\nu}^{xC}(s)$ are constant

$$\frac{d}{dt}m_{\mu}^{zC}(s) = 0, \quad (3.142)$$

$$\frac{d}{dt}m_{\nu}^{xC}(s) = 0, \quad (3.143)$$

and the solution of H_{op} is also given by $x_{i,j}^C(s), k_{i,j}^C(s), m_{\mu}^{zC}(s)$ and $m_{\nu}^{xC}(s)$. In addition, we find that this solution is simultaneously the solution of H_{op}^* because Eq. (3.48) is satisfied. Therefore, from uniqueness of the optimal control, this is just the solution of the motion of H_{op}^* , *i.e.*, the solution of the optimal control problem is given by

$$x_{i,j}^*(s) = x_{i,j}^C(s), \quad (3.144)$$

$$k_{i,j}^*(s) = k_{i,j}^C(s), \quad (3.145)$$

under the conditions of Eqs. (3.140) and (3.141). As a result, the optimal solution is equivalent to the static approximate solution and the static approximation is exact for the wide class of mean-field quantum spin systems (3.109).

3.5. Hidden classical nonlinear integrable systems in mean-field quantum spin systems

In this section, we focus on the property of the classical Hamiltonian, apart from mean-field quantum spin models. In general, it is a very difficult problem to solve nonlinear equations, except for classical nonlinear integrable systems. However, we could solve the nonlinear Hamilton's equations for the special initial and terminal conditions so far. Then, there is a natural question: does the classical Hamiltonian discussed in this thesis belong to classical nonlinear integrable systems? Or, is it accidental that we could write down the solution for special initial and terminal conditions? In the following, we show that the classical Hamiltonian discussed in this thesis belongs to classical nonlinear integrable systems.

3.5.1. Liouville integrability

Firstly, let us introduce the Liouville integrability. For a Hamiltonian system with n degrees of freedom $(x_1, \dots, x_n, k_1, \dots, k_n)$, we assume that there are n

first integrals of motion, H_1, \dots, H_n , which are independent of each other and in involution, that is,

$$\{H_i, H_j\} = \sum_{l=1}^N \left(\frac{\partial H_i}{\partial x_l} \frac{\partial H_j}{\partial k_l} - \frac{\partial H_i}{\partial k_l} \frac{\partial H_j}{\partial x_l} \right) = 0 \quad (i, j = 1, \dots, n). \quad (3.146)$$

where $\{, \}$ denotes the Poisson bracket. Then, the Liouville-Arnold theorem guarantees that the Hamilton's equations can be solved by a finite number of quadrature methods in principle, which is called the Liouville integrability.

3.5.2. Classical nonlinear integrable systems

Usually, it is an impossible task to solve nonlinear equations. Classical nonlinear integrable systems can be solved despite nonlinearity, and there is a miraculous mathematical trick behind. For example, the Toda lattice [48] is one of the most famous classical nonlinear integrable systems,

$$H = \frac{1}{2} \sum_{n=1}^N p_n^2 + \sum_{n=1}^N (e^{x_n - x_{n+1}} - 1). \quad (3.147)$$

Although this Hamilton's equations have nonlinearity, this system has N independent Poisson commuting invariants, that is, this system belongs to integrable system in the Liouville integrability. The Toda lattice can be solved by various methods, the inverse scattering method [112], the Hirota bilinear method [113] and the QR decomposition [114]. There are an infinite number of classical nonlinear integrable systems related to the Toda lattice and they are called the Toda hierarchy [49] (in the case of infinite degrees of freedom, the KP hierarchy [115, 116] is most famous.). However, to the best of our knowledge, the classical Hamiltonian discussed in this thesis is not included in the known classical nonlinear integrable systems.

3.5.3. Proof of integrability

In this subsection, we prove the Liouville integrability for the following classical Hamiltonian,

$$H_{\text{op}} = \sum_{\nu} g_{\nu} \left(\frac{\sum_{i,j,l} b_{i,l}^{\nu} x_{l,j} k_{i,j}}{\sum_{i,j} x_{i,j} k_{i,j}} \right) \sum_{i,j} x_{i,j} k_{i,j}, \quad (3.148)$$

$$\frac{dx_{i,j}}{dt} = x_{i,j} \left(\sum_{\nu} g_{\nu} - \sum_{\nu} g'_{\nu} m_{\nu} \right) + \sum_{\nu} g'_{\nu} \sum_l b_{i,l}^{\nu} x_{l,j}, \quad (3.149)$$

$$\frac{dk_{i,j}}{dt} = -k_{i,j} \left(\sum_{\nu} g_{\nu} - \sum_{\nu} g'_{\nu} m_{\nu} \right) - \sum_{\nu} g'_{\nu} \sum_l b_{i,l}^{\nu} k_{l,j}, \quad (3.150)$$

where g_ν is an arbitrary function with bracket as an argument and $b_{i,l}^\nu$ is an arbitrary real number satisfying $b_{l,i}^\nu = b_{i,l}^\nu$. This Hamiltonian contains the classical Hamiltonian which we have dealt with so far. Using $X_j \equiv (x_{1,j} \ x_{2,j} \ \cdots \ x_{N,j})^T$ and $K_j \equiv (k_{1,j} \ k_{2,j} \ \cdots \ k_{N,j})^T$, we can rewrite the Hamilton's equations as

$$H_{\text{op}} = \sum_\nu g_\nu \left(\frac{\sum_j K_j^T \hat{B}_\nu X_j}{\sum_j K_j^T X_j} \right) \sum_j K_j^T X_j, \quad (3.151)$$

$$\frac{d}{dt} X_j = \left(\sum_\nu g_\nu - \sum_\nu g'_\nu m_\nu \right) \hat{I} X_j + \sum_\nu g'_\nu \hat{B}_\nu X_j = \hat{C} X_j, \quad (3.152)$$

$$\frac{d}{dt} K_j = - \left(\sum_\nu g_\nu - \sum_\nu g'_\nu m_\nu \right) \hat{I} K_j - \sum_\nu g'_\nu \hat{B}_\nu K_j = -\hat{C} K_j, \quad (3.153)$$

$$\hat{C} \equiv \left(\sum_\nu g_\nu - \sum_\nu g'_\nu m_\nu \right) \hat{I} + \sum_\nu g'_\nu \hat{B}_\nu. \quad (3.154)$$

Then, this Hamiltonian can be regarded as a system in which N particles with N internal degrees of freedom interact.

Classical case: linear system

First, we consider the case where all of \hat{B}_ν commutes with each other, which corresponds to classical mean-field spin systems,

$$[\hat{C}, \hat{B}_\nu] = 0, \quad (3.155)$$

$$[\hat{B}_\nu, \hat{B}_{\nu'}] = 0. \quad (3.156)$$

Then, we find that m_ν is conserved because

$$\frac{d}{dt} m_\nu = - \frac{1}{\sum_j K_j^T X_j} \sum_j K_j^T [\hat{C}, \hat{B}_\nu] X_j = 0. \quad (3.157)$$

Therefore, the Hamilton's equations are reduced to linear equations, that is, the Hamiltonian belongs to linear integrable system.

Quantum case: nonlinear system

Next, we consider the case where \hat{B}_ν does not commute with each other, which corresponds to quantum mean-field spin systems. Then, m_ν is not preserved,

$$\frac{d}{dt} m_\nu = - \frac{1}{\sum_j K_j^T X_j} \sum_j K_j^T [\hat{C}, \hat{B}_\nu] X_j \neq 0, \quad (3.158)$$

and the Hamilton's equations are nonlinear equations. However, in the following, we will show that this Hamiltonian belongs to nonlinear integrable system using the fact that there are N^2 Poisson commuting invariants.

Firstly, we define $D_{i,j}$ as

$$D_{i,j} = X_i^T K_j = \sum_l x_{l,i} k_{l,j}. \quad (3.159)$$

From the Hamilton's equation, we find

$$\frac{d}{dt} D_{i,j} = \frac{d}{dt} (X_i^T) K_j + X_i^T \left(\frac{d}{dt} K_j \right) = X_i^T \hat{C} K_j - X_i^T \hat{C} K_j = 0. \quad (3.160)$$

Thus, we obtain N^2 preserved quantities. However, their Poisson brackets do not commute with each other,

$$\{D_{i,j}, D_{k,l}\} = \delta_{i,l} D_{k,j} - \delta_{j,k} D_{i,l} \neq 0. \quad (3.161)$$

Here, we define the $N^2 \times N^2$ square matrix \hat{D} as $(\hat{D})_{i,j} \equiv D_{i,j}$ and take the trace of \hat{D}^n ,

$$\begin{aligned} H_n &= \text{Tr}(\hat{D}^n) \\ &= \sum_{i_1, i_2, \dots, i_n} D_{i_1 i_2} D_{i_2 i_3} \cdots D_{i_{n-1} i_n} D_{i_n i_1} \\ &= \sum_{i_1, i_2, \dots, i_n} \sum_{l_1, l_2, \dots, l_n} x_{l_1, i_1} k_{l_1, i_2} x_{l_2, i_2} k_{l_2, i_3} \cdots x_{l_n, i_n} k_{l_n, i_1}, \end{aligned} \quad (3.162)$$

for $n = 1, 2, \dots, N^2$. Then, from Eq. (3.161), we find the following relation,

$$\{D_{i,j}, H_n\} = 0, \quad (3.163)$$

$$\{H_m, H_n\} = 0. \quad (3.164)$$

Therefore, we obtain the N^2 Poisson commuting invariants

$$H_n \quad (n = 1, 2, \dots, N^2). \quad (3.165)$$

In conclusion, the classical Hamiltonian discussed in this thesis belongs to nonlinear integrable system. To the best of our knowledge, the class of this classical nonlinear integrable system has not been known so far, that is, this system may be a new classical nonlinear integrable system. It is an intriguing future problem to solve this system for any initial conditions.

3.6. Conclusions

We have obtained the exact solution of the partition function for the particular class of mean-field quantum spin systems including randomness and showed that the static approximation is exact for these models in general. Although the imaginary-time dependence of the partition function of mean-field quantum spin systems had not been analyzed exactly, we gave a method to solve this problem exactly. Our result demonstrates that the method of the optimal control problem is a powerful approach to analysis of statistical mechanics.

As an application to quantum annealing, we verified exactness of the result of exponential speed up of quantum annealing by the non-stoquastic interaction or the inhomogeneous transverse field, which have recently attracted a lot of interest. Our analysis is an effective approach to quantum annealing by statistical mechanics.

In addition, we could introduce a new classical nonlinear integrable system by combining mean-field quantum systems and the optimal control theory. Our classical nonlinear integrable system has wide arbitrariness. The future problem is to solve the equations of motion for any initial conditions. Even though the Liouville integrability has been proved, it is not easy to actually find the solution of the Hamilton's equations. Furthermore, it is also a very exciting question what relation this system has to existing classical nonlinear integration systems.

In this chapter, we have shown that the static approximation is exact for the generalized Hopfield model with finite-number patterns and further generalization, which coincides with the prediction by Nishimori and Nonomura [85] as shown in Sec. 2.2.4. Nishimori and Nonomura also expected that the static approximation is broken for the Hopfield model with infinite-number patterns. Unfortunately, our method can not be applied to the Hopfield model with infinite-number patterns because we have to use the replica method. When we apply the replica method to the Hopfield model with infinite-number patterns, the partition function has a long-range imaginary-time interaction and we can not regard the partition function as the result of time evolution of the imaginary time Schrödinger equation. A similar difficulty also occurs for the p -spin-interacting spin glass model with the transverse field. Previous studies [76–84] showed that the static approximation gives a non-physical solution for the p -spin-interacting spin glass model with the transverse field in the paramagnetic phase. Although there are analyses based on the perturbation theory which incorporates the correction of the imaginary time dependence [80,83], it is hopeless to obtain the exact

solution at present. Essentially new developments are necessary, as Parisi [117] introduced the full replica symmetry breaking solution to the classical p -spin-interacting spin glass model. We hope that our method may be the first step to exactly analyze such system.

4. Quantum speed limit and classical speed limit

We have only considered equilibrium problems so far. Next, we consider dynamical property. Although it is very difficult to treat the time-dependent Schrödinger equation, there is an inequality which is called the quantum speed limit (QSL). The quantum speed limit, or the energy-time uncertainty relation, describes the fundamental maximum rate for quantum time evolution. The quantum speed limit is not only formal but also useful for practical purposes. Recent studies [40, 41] show that, using another type of quantum speed limit, the optimal computational time of the Grover problem in quantum annealing is order \sqrt{M} for the problem size M , which is consistent with the result of quantum circuit model.

The quantum speed limit was originally found in the context of the energy-time uncertainty relation [38] and, therefore, has been regarded as being unique in quantum mechanics. The main purpose of this chapter is to extend the quantum speed limit to classical systems and show that the quantum speed limit is not a purely quantum phenomenon but a universal dynamical property.

The relationship between the Heisenberg uncertainty principle and the quantum speed limit is explained in Sec 4.1. This section surveys previously known results on the quantum speed limit and, for later convenience, we reproduce the quantum speed limit for time-dependent quantum systems. In Sec 4.2, based on the Hilbert space for the classical Liouville equation, we derive a classical speed limit corresponding to the QSL. Thus, classical mechanics has a fundamental speed limit, and QSL is not a purely quantum phenomenon but a universal dynamical property of the Hilbert space, which is the main result of this chapter. We also obtain similar speed limits for the imaginary-time Schrödinger equations such as the classical master equation. Generalization to time-dependent systems is performed in Sec. 4.3 using the geometric method. Although the result of the geometric method is mathematically elegant, it is not suitable for actually evaluating its inequality in time-dependent systems. Section 4.4 introduces another

quantum speed limit which is called the Kieu bound [89]. The Kieu bound is suitable for evaluating its bound in time-dependent systems and was applied to the Grover problem in quantum annealing. Previous studies [40, 41] show that the optimal computational time is bounded from below by order \sqrt{M} , which is consistent with the previous study. In Sec. 4.5, we extend the Kieu bound to the imaginary-time Schrödinger equation. We show that the optimal computational time of the Grover problem in imaginary-time quantum annealing is bounded from below by order of $\log M$ for the problem size M , which is consistent with the result of a previous study [111].

This chapter is based on Refs. [118, 119].

4.1. Quantum speed limit

This section outlines the background of the subsequent studies. Section 4.1.1 discusses the relation between the Heisenberg's uncertainty principle and the quantum speed limit. We re-derive the quantum speed limit for time-independent systems in Sec. 4.1.2.

4.1.1. Heisenberg's uncertainty principle and quantum speed limit

Noncommutativity is one of the most important components of quantum mechanics. The Heisenberg's uncertainty principle [120]

$$\Delta x \Delta p \geq \frac{\hbar}{2} \quad (4.1)$$

stems from the canonical commutation relations [121]

$$[\hat{x}, \hat{p}] = i\hbar. \quad (4.2)$$

Because this consequence cannot appear in classical systems, Heisenberg's uncertainty principle is a purely quantum phenomenon. The product of energy and time has the same dimensions as the product of position and momentum, which naively implies the existence of a similar relation between energy and time. If there is a time operator \hat{T} which satisfies the canonical commutation relations for the Hamiltonian \hat{H}

$$[\hat{H}, \hat{T}] = i\hbar, \quad (4.3)$$

then we can obtain the energy-time uncertainty principle

$$\Delta E \Delta T \geq \frac{\hbar}{2}. \quad (4.4)$$

However, the time operator does not exist in a realistic model [122]. More specifically, it is proven that there is no time operator satisfying the canonical commutation relations for the Hamiltonian which has a lower bound on eigenvalues. Thus, there is no energy-time uncertainty principle that strictly corresponds to Heisenberg's uncertainty principle. Properly formulating the uncertainty relation for energy and time is a delicate issue that is still being discussed [123, 124].

The first rigorous derivation of an analogous uncertainty principle for energy and time was given by Mandelstam and Tamm [38], in which they determined that the product of the energy variance ΔE and time τ required for a state to be orthogonal to its initial state was greater than Planck's constant,

$$\tau \geq \tau_{\text{QSL}} = \frac{\pi \hbar}{2 \Delta E}. \quad (4.5)$$

This result implied that quantum mechanics has a fundamental speed limit characterized by Planck's constant, and thus, this inequality is called the energy-time uncertainty relation or quantum speed limit (QSL). The quantum speed limit can also be regarded as a trade-off between energy and time in the variance of a state. Investigating the restrictions on the time evolution of quantum dynamics is an interesting and important problem, and there are many related works: the Margolus–Levitin bound [39], the shortest time for quantum computation [90], cases on mixed states [91], time-dependent systems [45, 92, 93], and open systems [94–96], geometric derivations of the QSL [97–101], and various applications [102–109].

4.1.2. Quantum speed limit

Let us introduce two representative studies: the Mandelstam–Tamm bound and the Margolus–Levitin bound.

We consider the time-independent Hamiltonian \hat{H} . The state $|\phi(t)\rangle$ of the system satisfies the Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t} |\phi(t)\rangle = \hat{H} |\phi(t)\rangle. \quad (4.6)$$

Then, the minimal evolution time τ_{QSL} needed for the state to rotate orthogonally is bounded as [38],

$$\tau \geq \tau_{\text{QSL}} = \frac{\pi \hbar}{2 \Delta E}, \quad (4.7)$$

where ΔE is the energy variance defined as $\sqrt{\langle \phi | \hat{H}^2 | \phi \rangle - \langle \phi | \hat{H} | \phi \rangle^2}$. This inequality is known as the Mandelstam–Tamm bound.

Another quantum speed limit, which is called the Margolus–Levitin bound [39], is given by

$$\tau \geq \tau_{\text{QSL}} = \frac{\pi \hbar}{2(E - E_0)}, \quad (4.8)$$

where E is the mean energy $\langle \phi | \hat{H} | \phi \rangle$ and E_0 is the ground-state energy.

In general, these speed limits are independent, and thus, the minimal evolution time is restricted as follows:

$$\tau \geq \tau_{\text{QSL}} = \max \left\{ \frac{\pi \hbar}{2\Delta E}, \frac{\pi \hbar}{2(E - E_0)} \right\}. \quad (4.9)$$

In the following, based on Ref. [91], we reproduce the Mandelstam–Tamm bound and the Margolus–Levitin bound including non-orthogonal states. This procedure will grasp the understanding of the quantum speed limit and lead us to the classical speed limit in the next section.

Derivation of the Margolus-Levitin bound

First, we obtain the Margolus-Levitin bound. We assume that the ground-state energy E_0 is equal to 0

$$\hat{H}|n\rangle = E_n|n\rangle, \quad (4.10)$$

$$E_0 = 0. \quad (4.11)$$

For a given initial state $|\phi\rangle$

$$|\phi\rangle = \sum_n c_n |n\rangle, \quad (4.12)$$

the overlap $P(t)$ between $|\phi\rangle$ and $|\phi(t)\rangle$ following the Schrödinger equation is given by

$$P(t) = |\langle \psi | \psi(t) \rangle|^2 = \left| \sum_n |c_n|^2 e^{-iE_n t/\hbar} \right|^2. \quad (4.13)$$

We consider the case where $P(t)$ is equal to ϵ . From the definition of $\langle \psi | \psi(t) \rangle$

$$\langle \psi | \psi(t) \rangle = \sqrt{\epsilon} e^{i\theta} = \sum_n |c_n|^2 e^{-iE_n t/\hbar}, \quad (4.14)$$

we obtain the following relations

$$\sum_n |c_n|^2 \cos \frac{E_n t}{\hbar} = \sqrt{\epsilon} \cos \theta, \quad (4.15)$$

$$\sum_n |c_n|^2 \sin \frac{E_n t}{\hbar} = -\sqrt{\epsilon} \sin \theta. \quad (4.16)$$

The key point is the following inequality

$$\cos x + q \sin x \geq 1 - ax \quad (x \geq 0), \quad (4.17)$$

where a and q satisfy

$$a = \frac{y + \sqrt{y^2(1+q^2) + q^2}}{1+y^2}, \quad (4.18)$$

$$\sin y = \frac{a(1-xy) + q}{1+q^2}. \quad (4.19)$$

Setting $x = E_n t / \hbar$, we find

$$\cos \frac{E_n t}{\hbar} + q \sin \frac{E_n t}{\hbar} \geq 1 - a \frac{E_n t}{\hbar}. \quad (4.20)$$

By multiplying $|c_n|^2$ and summing over n , we get the following expression

$$\sqrt{\epsilon}(\cos \theta - q \sin \theta) \geq 1 - a \frac{Et}{\hbar}, \quad (4.21)$$

$$\begin{aligned} \Leftrightarrow t &\geq \frac{\hbar}{aE} [1 - \sqrt{\epsilon}(\cos \theta - q \sin \theta)] \\ &= [1 - \sqrt{\epsilon}(\cos \theta - q \sin \theta)] \frac{1}{a} \frac{\hbar}{E}. \end{aligned} \quad (4.22)$$

This is the Margolus-Levitin bound including the case where the two states are not orthogonal. This inequality means that the minimum time τ_{QSL} required for the overlap to be ϵ is limited

$$\tau_{QSL}(\epsilon) = \alpha(\epsilon) \frac{\hbar}{E} \quad (4.23)$$

$$\alpha(\epsilon) \equiv \min_{\theta} \left\{ \max_q \left\{ [1 - \sqrt{\epsilon}(\cos \theta - q \sin \theta)] \frac{1}{a} \right\} \right\} \quad (4.24)$$

When $\epsilon = 0$, this inequality is reduced to the orthogonal case.

Derivation of the Mandelstam-Tamm bound

Next, we reproduce the Mandelstam-Tamm bound. We take derivative of $P(t)$ with respect to t ,

$$\begin{aligned}
\frac{dP(t)}{dt} &= \frac{1}{\hbar} \sum_m \sum_n |c_n|^2 |c_m|^2 (-iE_n + iE_m) e^{iE_m t/\hbar - iE_n t/\hbar} \\
&= \frac{1}{\hbar} \sum_m \sum_n |c_n|^2 |c_m|^2 (-iE_n) (e^{iE_m t/\hbar - iE_n t/\hbar} - e^{-iE_m t/\hbar + iE_n t/\hbar}) \\
&= \frac{2}{\hbar} \sum_m \sum_n |c_n|^2 |c_m|^2 E_n \sin\left(\frac{E_m t}{\hbar} - \frac{E_n t}{\hbar}\right) \\
&= \frac{2}{\hbar} \sum_m \sum_n |c_n|^2 |c_m|^2 (E_n - E) \sin\left(\frac{E_m t}{\hbar} - \frac{E_n t}{\hbar}\right), \tag{4.25}
\end{aligned}$$

where we used $\sum_m \sum_n |c_n|^2 |c_m|^2 \sin\left(\frac{E_m t}{\hbar} - \frac{E_n t}{\hbar}\right) = 0$ in the last equality. Then, taking the absolute value, we obtain

$$\begin{aligned}
\left| \frac{dP(t)}{dt} \right| &= \left| \frac{2}{\hbar} \sum_m \sum_n |c_n|^2 |c_m|^2 (E_n - E) \sin\left(\frac{E_n t}{\hbar} - \frac{E_m t}{\hbar}\right) \right| \\
&\leq \left| \frac{2}{\hbar} \sum_m \sum_n |c_n|^2 |c_m|^2 (E_n - E) e^{-i\frac{E_n t}{\hbar} + i\frac{E_m t}{\hbar}} \right| \\
&= \left| \frac{2}{\hbar} \sum_n |c_n|^2 (E_n - E) \left(\sum_m |c_m|^2 e^{-i\frac{E_n t}{\hbar} + i\frac{E_m t}{\hbar}} - P(t) \right) \right|, \tag{4.26}
\end{aligned}$$

where we added a constant using $\sum_n |c_n|^2 |c_m|^2 (E_n - E) = 0$ in the last equality. Furthermore, using the Cauchy-Schwartz inequality, we find

$$\begin{aligned}
\left| \frac{dP(t)}{dt} \right| &\leq \left| \frac{2}{\hbar} \sum_n c_n^* (E_n - E) \left\{ c_n \left(\sum_m |c_m|^2 e^{-i\frac{E_n t}{\hbar} + i\frac{E_m t}{\hbar}} - P(t) \right) \right\} \right| \\
&\leq \frac{2}{\hbar} \sqrt{\sum_n |c_n^* (E_n - E)|^2} \sqrt{\sum_n \left| c_n \left(\sum_m |c_m|^2 e^{-i\frac{E_n t}{\hbar} + i\frac{E_m t}{\hbar}} - P(t) \right) \right|^2} \\
&= \frac{2}{\hbar} \Delta E \sqrt{P(t)[1 - P(t)]}. \tag{4.27}
\end{aligned}$$

Finally, the following relation

$$\frac{d}{dx} (\arccos \sqrt{x}) = \frac{1}{2\sqrt{x}} \frac{1}{\sqrt{1-x}} = \frac{1}{2\sqrt{x(1-x)}} \tag{4.28}$$

leads to

$$\frac{d}{dt} \arccos \sqrt{P(t)} \leq \frac{\Delta E}{\hbar} \tag{4.29}$$

Therefore, we obtain the Mandelstam-Tamm bound including the case where the two states are not orthogonal,

$$\tau \geq \tau_{QSL}(\epsilon) = \arccos \sqrt{\epsilon} \frac{\hbar}{\Delta E} \tag{4.30}$$

4.2. Classical speed limit

Note that the QSL is a strictly different concept than Heisenberg's uncertainty principle. Nevertheless, since QSL appears in a similar context to Heisenberg's uncertainty principle, QSL has been considered a purely quantum phenomenon with no corresponding concept in classical mechanics. Recent studies [42–45] have argued that QSL vanishes in the classical limit, and the time evolution of classical mechanics has no fundamental speed limit. However, in this section, we show that a fundamental speed limit exists even in classical mechanics. Inspired by the fact that QSL was obtained from the Hilbert space for the Schrödinger equation as shown in the previous section, we utilized a similar analysis on the classical Liouville equation [125,126]. We rigorously proved that classical mechanics also has a fundamental speed limit, namely, the classical speed limit (CSL). As a result, we concluded that QSL is not a particular phenomenon to quantum mechanics; instead, QSL is a universal property of the time evolution of the Hilbert space. Furthermore, this method was applied to the imaginary-time Schrödinger equation, e.g., the Fokker–Planck equation and the classical master equation, and we showed that these equations also have fundamental speed limits.

First, we introduce the Hilbert space for the classical Liouville equation in Sec. 4.2.1. Section 4.2.2 is devoted to obtaining the classical speed limit corresponding to the Margolus–Levitin bound. In Sec. 4.2.3, we obtain the Mandelstam–Tamm-type bound for the classical Liouville equation. We show that the imaginary-time Schrödinger equation also has a similar speed limit in Sec. 4.2.4.

4.2.1. Hilbert space for the classical Liouville equation

Consider the time-independent classical Hamiltonian $H(\mathbf{z})$, where $\mathbf{z} = (x_1, \dots, x_N, p_1, \dots, p_N)$ specifies a point in the N -dimensional phase space and $H(\mathbf{z})$ belongs to an integrable or nonintegrable system. The evolution of the phase space distribution $\rho(\mathbf{z}, t)$ obeys the classical Liouville equation,

$$i \frac{\partial \rho(\mathbf{z}, t)}{\partial t} = \hat{L} \rho(\mathbf{z}, t) \equiv i \{H(\mathbf{z}), \rho(\mathbf{z}, t)\}, \quad (4.31)$$

where $\{\cdot, \cdot\}$ denotes the Poisson bracket, \hat{L} is called the Liouvillian, and $\rho(\mathbf{z}, t)$ is normalized as $\int d\mathbf{z} \rho(\mathbf{z}, t) = 1$. The Liouvillian is a Hermitian operator with respect to the given inner product $\langle \rho_1 | \rho_2 \rangle \equiv \int d\mathbf{z} \rho_1^*(\mathbf{z}) \rho_2(\mathbf{z})$ (see appendix D for a proof). Then, using the eigenstate $|n\rangle$ of \hat{L} , we can expand $\rho(\mathbf{z}, t)$ as

$$|\rho(t)\rangle = \sum_n c_n e^{-i\lambda_n t} |n\rangle, \quad (4.32)$$

where c_n is a time-independent constant and $\langle \rho(t) | \rho(t) \rangle \neq 1$. We note that $\langle \rho | \hat{L} | \rho \rangle = 0$ and, if λ_n is an eigenvalue of \hat{L} , then $-\lambda_n$ is also an eigenvalue of \hat{L} (see appendix D for a proof).

In the following, we obtain the CSL for the classical Liouville equation by using the Hilbert space for the classical Liouville equation.

4.2.2. Derivation of the ML-type bound for the classical Liouville equation

First, we obtain the CSL corresponding to the Margolus–Levitin bound (4.8). We consider the overlap between the initial state $|\rho\rangle$ and the final state $|\rho(t)\rangle$. We evaluate $\langle \rho | \rho(t) \rangle$ as

$$\begin{aligned} \langle \rho | \rho(t) \rangle &= \sum |c_n|^2 \cos(\lambda_n t) \\ &\geq \sum |c_n|^2 \left(1 - \frac{\lambda_n^2 t^2}{2} \right), \end{aligned} \quad (4.33)$$

where we use $\cos x \geq 1 - x^2/2$ and $\langle \rho | \rho(t) \rangle$ takes a real value. From Eq. (4.33), we obtain CSL for the classical Liouville equation,

$$\tau \geq \tau_{\text{CSL}} = \sqrt{\frac{2(\langle \rho | \rho \rangle - \langle \rho | \rho(\tau) \rangle)}{\langle \rho | \hat{L}^2 | \rho \rangle}}. \quad (4.34)$$

This means that the classical time development is also restricted, and there is a trade-off between the classical Hamiltonian (or the Liouvillian) and time during time evolution of the phase space distribution.

From the derivation, this CSL corresponds to the Margolus–Levitin bound in quantum systems [39, 91]. However, we note that we cannot use an odd function for evaluating the inequality because eigenvalues λ_n always take symmetric positive and negative values, unlike quantum systems. For this reason, the form of the CLS is different than the Margolus–Levitin bound (4.8) in quantum systems.

We stress that QSL and CSL are derived not from noncommutativity; they are dynamical properties of the Hilbert space. This implies that there are general fundamental speed limits for time-evolution systems. Later, we will show that several stochastic equations also have similar speed limits.

Up to now, we have considered many-particle movement following the same Hamiltonian. Next, let us consider the single particle limit of CSL. For example,

we consider the one-dimensional harmonic oscillator,

$$\rho(x, p, 0) = \frac{\sqrt{ab}}{\pi} e^{-a(x-e)^2 - b(p-f)^2}, \quad (4.35)$$

$$H(x, p) = dp^2 + cx^2, \quad (4.36)$$

where $\int dx \int dp \rho(x, p) = 1$, $d = 1/(2m)$, and $c = m\omega^2/2$. After straightforward calculations, we obtain

$$\langle \rho | \hat{L}^2 | \rho \rangle = \frac{(ad - bc)^2 + 4a^2bd^2f^2 + 4ab^2c^2e^2}{2\pi\sqrt{ab}}. \quad (4.37)$$

Taking the limit $a, b \rightarrow \infty$, Eq. (4.35) goes to the δ function, which means that the particles are only at one point in the phase space, that is, the single particle limit. Then, we find that the right hand side of Eq. (4.34) goes to zero and CSL vanishes. This means that CSL is essentially an effect of many particles in classical systems, which is a natural consequence, because we cannot define the overlap of the phase space distribution for single particles in classical mechanics.

Although $\langle \rho | \rho \rangle$ has not been normalized, we can adjust it using the fact that the square root of $\rho(\mathbf{z}, t)$ also satisfies the Liouville equation,

$$i \frac{\partial \rho^{1/2}(\mathbf{z}, t)}{\partial t} = \hat{L} \rho^{1/2}(\mathbf{z}, t). \quad (4.38)$$

This enables us to expand $\rho^{1/2}(\mathbf{z}, t)$ as $|\rho^{(1/2)}(t)\rangle = \sum_n c_n^{(1/2)} e^{-i\lambda_n t} |n\rangle$, where $c_n^{(1/2)}$ is a time-independent constant and $\langle \rho^{(1/2)}(t) | \rho^{(1/2)}(t) \rangle = 1$. Using the same technique as before, we obtain another speed limit for the classical Liouville equation,

$$\tau \geq \tau_{\text{CSL}}^{(1/2)} = \sqrt{\frac{2(1 - \langle \rho^{1/2} | \rho^{1/2}(\tau) \rangle)}{\langle \rho^{1/2} | \hat{L}^2 | \rho^{1/2} \rangle}}. \quad (4.39)$$

Furthermore, we immediately find that $\rho^\alpha(\mathbf{z}, t)$ satisfies

$$i \frac{\partial \rho^\alpha(\mathbf{z}, t)}{\partial t} = \hat{L} \rho^\alpha(\mathbf{z}, t), \quad (4.40)$$

and can be expanded as $|\rho^{(\alpha)}(t)\rangle = \sum_n c_n^{(\alpha)} e^{-i\lambda_n t} |n\rangle$, where α is any real value and $c_n^{(\alpha)}$ is a time-independent constant. Thus, we obtain an infinite number of classical speed limits,

$$\tau \geq \tau_{\text{CSL}}^{(\alpha)} = \sqrt{\frac{2(\langle \rho^{(\alpha)} | \rho^{(\alpha)} \rangle - \langle \rho^{(\alpha)} | \rho^{(\alpha)}(\tau) \rangle)}{\langle \rho^{(\alpha)} | \hat{L}^2 | \rho^{(\alpha)} \rangle}}. \quad (4.41)$$

For a given phase space distribution and Hamiltonian, these speed limits always hold. Note that these inequalities for different parameters between α and α' are independent and cannot be generally ordered in tightness.

4.2.3. Derivation of MT-type bound for classical Liouville equation

Next, we obtain the Mandelstam–Tamm-type bound for the classical Liouville equation. We take the derivative of $\langle \rho^{(\alpha)} | \rho^{(\alpha)}(t) \rangle$ with respect to t ,

$$\begin{aligned} \left| \frac{d\langle \rho^{(\alpha)} | \rho^{(\alpha)}(t) \rangle}{dt} \right| &= \left| \sum_n |c_n^{(\alpha)}|^2 \lambda_n \sin(\lambda_n t) \right| \\ &\leq \left| \sum_n |c_n^{(\alpha)}|^2 \lambda_n e^{-i\lambda_n t} \right| \\ &= \left| \sum_n |c_n^{(\alpha)}|^2 \lambda_n \left(e^{-i\lambda_n t} - \frac{\langle \rho^{(\alpha)} | \rho^{(\alpha)}(t) \rangle}{\langle \rho^\alpha | \rho^\alpha \rangle} \right) \right|, \end{aligned} \quad (4.42)$$

where we used $\sum_n |c_n^{(\alpha)}|^2 \lambda_n = \langle \rho^{(\alpha)} | \hat{L} | \rho^{(\alpha)} \rangle = 0$ in the last identity. Furthermore, the Cauchy–Schwarz inequality leads to

$$\begin{aligned} \left| \frac{d\langle \rho^{(\alpha)} | \rho^{(\alpha)}(t) \rangle}{dt} \right| &\leq \sqrt{\langle \rho^{(\alpha)} | \hat{L}^2 | \rho^{(\alpha)} \rangle} \\ &\quad \sqrt{\langle \rho^\alpha | \rho^\alpha \rangle - \frac{\langle \rho^{(\alpha)} | \rho^{(\alpha)}(t) \rangle^2}{\langle \rho^\alpha | \rho^\alpha \rangle}}. \end{aligned} \quad (4.43)$$

Therefore, we obtain another CSL

$$\tau \geq \tau_{\text{CSL}}^{(\alpha)} = \frac{\arccos \frac{\langle \rho^{(\alpha)} | \rho^{(\alpha)}(\tau) \rangle}{\langle \rho^{(\alpha)} | \rho^{(\alpha)} \rangle}}{\sqrt{\frac{\langle \rho^{(\alpha)} | \hat{L}^2 | \rho^{(\alpha)} \rangle}{\langle \rho^{(\alpha)} | \rho^{(\alpha)} \rangle}}}. \quad (4.44)$$

This CSL corresponds to the Mandelstam–Tamm bound in quantum systems [39, 91] from the derivation. We note that the denominator of Eq. (4.44) is equivalent to the average standard deviation of \hat{L} because $\langle \rho^{(\alpha)} | \hat{L} | \rho^{(\alpha)} \rangle = 0$.

Although it is not possible to compare the speed limits Eqs. (4.7) and (4.8) in quantum systems, we can compare two speed limits Eqs. (4.41) and (4.44) in classical systems. We immediately find

$$\tau \geq \frac{\arccos \frac{\langle \rho^{(\alpha)} | \rho^{(\alpha)}(\tau) \rangle}{\langle \rho^{(\alpha)} | \rho^{(\alpha)} \rangle}}{\sqrt{\frac{\langle \rho^{(\alpha)} | \hat{L}^2 | \rho^{(\alpha)} \rangle}{\langle \rho^{(\alpha)} | \rho^{(\alpha)} \rangle}}} \geq \sqrt{\frac{2 \left(1 - \frac{\langle \rho^{(\alpha)} | \rho^{(\alpha)}(\tau) \rangle}{\langle \rho^{(\alpha)} | \rho^{(\alpha)} \rangle} \right)}{\frac{\langle \rho^{(\alpha)} | \hat{L}^2 | \rho^{(\alpha)} \rangle}{\langle \rho^{(\alpha)} | \rho^{(\alpha)} \rangle}}}. \quad (4.45)$$

Therefore, in classical system, the Mandelstam–Tamm-type bound (4.44) is the better classical speed limit than the Margolus–Levitin-type bound (4.41).

4.2.4. Speed limit for the imaginary-time Schrödinger equation

Although we have considered only the classical Liouville equation, the system has been represented by the Hilbert space. In other words, if the time evolution is expressed using a Hermitian operator, it can be expected that the system would have a similar speed limit.

First, let us consider the Fokker–Planck equation,

$$\frac{\partial}{\partial t} P(x, t) = \frac{\partial}{\partial x} \left[\left(2 \frac{\partial W(x)}{\partial x} + \frac{\partial}{\partial x} \right) P(x, t) \right]. \quad (4.46)$$

This equation has a stationary solution $P_0(x) = \exp(-2W(x))$. Using $P(x, t) = \exp(-W(x))\psi(x, t)$, we obtain the imaginary-time Schrödinger equation,

$$\begin{aligned} -\frac{\partial}{\partial t} \psi(x, t) &= \left[-\frac{\partial^2}{\partial x^2} + \left(\frac{\partial W(x)}{\partial x} \right)^2 - \frac{\partial^2 W(x)}{\partial x^2} \right] \psi(x, t) \\ &\equiv \hat{H}_F \psi(x, t). \end{aligned} \quad (4.47)$$

Then, the ground state of \hat{H}_F is given by $\phi_0(x, t) = \exp(-W(x))$, which has the ground state eigenvalue $E_0 = 0$, and the eigenvalues of the excited states are always positive $E_n > 0$. Using the eigenstates $|\psi_n\rangle$ of \hat{H}_F , we expand the state $\psi(x, t)$ as $|\psi(t)\rangle = \sum_n d_n e^{-E_n t} |\psi_n\rangle$, where d_n is a time-independent constant. Then, we evaluate $\langle \psi | \psi(t) \rangle / \langle \psi | \psi \rangle$ as

$$\begin{aligned} \frac{\langle \psi | \psi(t) \rangle}{\langle \psi | \psi \rangle} &= \sum_n \frac{|d_n|^2}{\langle \psi | \psi \rangle} e^{-E_n t} \\ &\geq \exp \left(-\sum_n \frac{|d_n|^2}{\langle \psi | \psi \rangle} E_n t \right) \\ &= \exp \left(-t \frac{\langle \psi | \hat{H}_F | \psi \rangle}{\langle \psi | \psi \rangle} \right). \end{aligned} \quad (4.48)$$

where we use Jensen’s inequality. Therefore, we obtain a speed limit corresponding to the Margolus–Levitin bound (4.8) for the Fokker–Planck equation:

$$\tau \geq \tau_{\min} = \frac{\log \langle \psi | \psi \rangle - \log \langle \psi | \psi(\tau) \rangle}{\frac{\langle \psi | \hat{H}_F | \psi \rangle}{\langle \psi | \psi \rangle}}. \quad (4.49)$$

Next, we obtain the speed limit corresponding to the Mandelstam–Tamm bound (4.7) for the Fokker–Planck equation. We take the derivative of $\langle \psi | \psi(t) \rangle$

with respect to t ,

$$\begin{aligned} -\frac{d}{dt}\langle\psi|\psi(t)\rangle &= \sum_n |d_n|^2 E_n e^{-E_n t} \\ &\leq \sum_n |d_n|^2 E_n e^{-E_n t/2}. \end{aligned} \quad (4.50)$$

Applying the Cauchy–Schwarz inequality, we get

$$-\frac{d}{dt}\langle\psi|\psi(t)\rangle \leq \sqrt{\langle\psi|\hat{H}_F^2|\psi\rangle} \sqrt{\langle\psi|\psi(t)\rangle}. \quad (4.51)$$

Therefore, we find the speed limit

$$\tau \geq \tau_{\min} = 2 \frac{\sqrt{\langle\psi|\psi\rangle} - \sqrt{\langle\psi|\psi(\tau)\rangle}}{\sqrt{\langle\psi|\hat{H}_F^2|\psi\rangle}}. \quad (4.52)$$

We note that Eqs. (4.49) and (4.52) are generally independent, and thus, the speed limit for the Fokker–Planck equation is given by

$$\tau_{\min} = \max \left(\frac{\log \frac{\langle\psi|\psi\rangle}{\langle\psi|\psi(\tau)\rangle}}{\frac{\langle\psi|\hat{H}_F|\psi\rangle}{\langle\psi|\psi\rangle}}, \frac{2 - 2\sqrt{\frac{\langle\psi|\psi(\tau)\rangle}{\langle\psi|\psi\rangle}}}{\sqrt{\frac{\langle\psi|\hat{H}_F^2|\psi\rangle}{\langle\psi|\psi\rangle}}} \right). \quad (4.53)$$

Finally, we consider the classical master equation and assume that the detailed balance condition holds,

$$\frac{d}{dt}P(t) = -\hat{W}P(t). \quad (4.54)$$

Then, the transition matrix \hat{W} can be represented by a symmetric matrix, and its eigenvalues λ_n satisfy $0 = \lambda_0 < \lambda_1 < \lambda_2 < \dots < \lambda_N$. Therefore, using the eigenstates $|n\rangle$ of W , we can expand the probability $P(t)$ as $|P(t)\rangle = \sum_n e_n e^{-\lambda_n t} |n\rangle$ and obtain the speed limit for the classical master equation:

$$\tau_{\min} = \max \left(\frac{\log \frac{\langle P|P\rangle}{\langle P|P(\tau)\rangle}}{\frac{\langle P|\hat{W}|P\rangle}{\langle P|P\rangle}}, \frac{2 - 2\sqrt{\frac{\langle P|P(\tau)\rangle}{\langle P|P\rangle}}}{\sqrt{\frac{\langle P|\hat{W}^2|P\rangle}{\langle P|P\rangle}}} \right). \quad (4.55)$$

This is the fundamental speed limit for the classical master equation. We note that, if the detailed balance condition is broken, we cannot obtain a similar fundamental speed limit because the probability cannot be expanded using the eigenstates of W .

4.3. Generalization to time-dependent systems

We have obtained the classical speed limit for time-independent systems so far. On the other hand, the quantum speed limit was generalized to time-dependent systems using a geometric method [97, 101]. In this section, following this standard procedure, we also generalize the classical speed limit to time-dependent systems.

The classical Liouville equation describes the time evolution in the Hilbert space and the norm of the state is always constant, which means that the state is moving on the spherical surface. Then, as a distance between two differential states on the spherical surface, it is natural to use the Bures distance L

$$L(0, t) \equiv \arccos \left(\frac{\langle \rho^{(\alpha)} | \rho^{(\alpha)}(t) \rangle}{\sqrt{\langle \rho^{(\alpha)} | \rho^{(\alpha)} \rangle \langle \rho^{(\alpha)}(t) | \rho^{(\alpha)}(t) \rangle}} \right). \quad (4.56)$$

It is known that the Bures distance satisfies the triangle inequality

$$L(t_1, t_2) + L(t_2, t_3) \geq L(t_1, t_3). \quad (4.57)$$

Taking the Bures distance between t and $t + dt$ for $dt \ll 1$, we obtain

$$(L(t, t + dt))^2 = \frac{\langle d\rho^{(\alpha)}(t) | d\rho^{(\alpha)}(t) \rangle}{\langle \rho^{(\alpha)}(t) | \rho^{(\alpha)}(t) \rangle} - \frac{\langle \rho^{(\alpha)}(t) | d\rho^{(\alpha)}(t) \rangle \langle d\rho^{(\alpha)}(t) | \rho^{(\alpha)}(t) \rangle}{\langle \rho^{(\alpha)}(t) | \rho^{(\alpha)}(t) \rangle^2}. \quad (4.58)$$

Using the classical Liouville equation and $\langle \rho^{(\alpha)}(t) | \hat{L}(t) | \rho^{(\alpha)}(t) \rangle = 0$, we obtain

$$(L(t, t + dt))^2 = \frac{\langle \rho^{(\alpha)}(t) | \hat{L}^2(t) | \rho^{(\alpha)}(t) \rangle}{\langle \rho^{(\alpha)}(t) | \rho^{(\alpha)}(t) \rangle} dt^2. \quad (4.59)$$

Then, the total length $l_{0 \rightarrow \gamma}$ of the motion trajectory on the spherical surface is given by

$$l_{0 \rightarrow \gamma} = \int_0^\tau L(t, t + dt) = \int_0^\tau dt \sqrt{\frac{\langle \rho^{(\alpha)}(t) | \hat{L}^2(t) | \rho^{(\alpha)}(t) \rangle}{\langle \rho^{(\alpha)}(t) | \rho^{(\alpha)}(t) \rangle}}. \quad (4.60)$$

Furthermore, the triangle inequality for the Bures distance leads to

$$l_{0 \rightarrow \gamma} \geq L(0, \tau). \quad (4.61)$$

Therefore, CSL for the time-dependent Liouville equation is given by

$$\tau \geq \frac{\arccos \left(\frac{\langle \rho^{(\alpha)} | \rho^{(\alpha)}(\tau) \rangle}{\sqrt{\langle \rho^{(\alpha)} | \rho^{(\alpha)} \rangle \langle \rho^{(\alpha)}(\tau) | \rho^{(\alpha)}(\tau) \rangle}} \right)}{\frac{1}{\tau} \int_0^\tau dt \sqrt{\frac{\langle \rho^{(\alpha)}(t) | \hat{L}^2(t) | \rho^{(\alpha)}(t) \rangle}{\langle \rho^{(\alpha)}(t) | \rho^{(\alpha)}(t) \rangle}}}. \quad (4.62)$$

In the case where the Hamiltonian is time-independent, E.q. (4.62) is deduced to Eq. (4.44).

Similar analysis can be applied to the imaginary-time Schrödinger equation,

$$-\frac{d}{dt}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle, \quad (4.63)$$

and we immediately obtain the following inequality

$$\tau \geq \frac{\arccos\left(\frac{\langle\psi|\psi(\tau)\rangle}{\sqrt{\langle\psi|\psi\rangle\langle\psi(\tau)|\psi(\tau)\rangle}}\right)}{\frac{1}{\tau}\int_0^\tau dt\sqrt{\frac{\langle\psi(t)|\hat{H}^2(t)|\psi(t)\rangle}{\langle\psi(t)|\psi(t)\rangle} - \left(\frac{\langle\psi(t)|\hat{H}(t)|\psi(t)\rangle}{\langle\psi(t)|\psi(t)\rangle}\right)^2}}. \quad (4.64)$$

4.4. A useful speed limit for the real-time Schrödinger equation

Although the result of QSL are mathematically elegant, it is, in general, very difficult to evaluate the bound for a given time-dependent Hamiltonian and initial state because it requires information on the intermediate state of time evolution. On the other hand, there is another class of QSL and it is not only formal but also suitable for actually evaluating the speed limit [41, 89, 93]. For example, for a given Hamiltonian $\hat{H}(t)$, the initial state $|\psi_0\rangle$ and the state $|\psi(\tau)\rangle$ following the Schrödinger equation, Kieu [89] derived the following inequality

$$\hbar\| |\psi(\tau)\rangle - e^{-i\int_0^\tau ds\alpha(s)}|\psi_0\rangle\| \leq \int_0^\tau dt\|(\hat{H}(t) - \alpha(t))|\psi_0\rangle\|, \quad (4.65)$$

where $\alpha(t)$ is a time-dependent arbitrary function. Note that Eq. (4.65) contains only the initial state and a given Hamiltonian, and does not require the information on the intermediate state of the dynamics. This enables us to easily evaluate the right hand side of Eq. (4.65). In addition, Eq. (4.65) is not only computable but also tight. Recent study [40, 41] shows that, using Eq. (4.65), the optimal computational time of the Grover problem [50, 57] is order \sqrt{M} for the problem size M in quantum annealing [6, 12].

In this section, we review the result of Ref. [89].

4.4.1. Derivation of the Kieu bound

We consider two real-time Schrödinger equations,

$$i\partial_t|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle, \quad (4.66)$$

$$i\partial_t|\phi(t)\rangle = \alpha(t)\mathbf{1}|\phi(t)\rangle, \quad (4.67)$$

$$|\psi(0)\rangle = |\phi(0)\rangle = |\psi_0\rangle, \quad (4.68)$$

where $\alpha(t)$ is a time-dependent arbitrary function and $\mathbf{1}$ is the identity matrix. Taking the difference between Eqs. (4.66) and (4.67), we obtain

$$\hbar\partial_t(|\psi(t)\rangle - |\phi(t)\rangle) = -i\hat{H}(t)(|\psi(t)\rangle - |\phi(t)\rangle) - i(\hat{H}(t) - \alpha(t))|\phi(t)\rangle. \quad (4.69)$$

Considering the distance between $|\psi(t)\rangle$ and $|\phi(t)\rangle$, we obtain

$$\begin{aligned} \hbar\partial_t\| |\psi(t)\rangle - |\phi(t)\rangle \|^2 &= \hbar(\langle\psi(t)| - \langle\phi(t)|) \cdot \partial_t(|\psi(t)\rangle - |\phi(t)\rangle) \\ &\quad + \hbar\{\partial_t(\langle\psi(t)| - \langle\phi(t)|)\}(|\psi(t)\rangle - |\phi(t)\rangle) \\ &= 2\hbar\Re(\langle\psi(t)| - \langle\phi(t)|)\partial_t(|\psi(t)\rangle - |\phi(t)\rangle). \end{aligned} \quad (4.70)$$

Substituting Eq. (4.69) into Eq. (4.70), we obtain

$$\begin{aligned} \hbar\partial_t\| |\psi(t)\rangle - |\phi(t)\rangle \|^2 &= 2\Im(\langle\psi(t)| - \langle\phi(t)|)(\hat{H}(t) - \alpha(t))|\phi(t)\rangle) \\ &\leq 2\| |\psi(t)\rangle - |\phi(t)\rangle \| \cdot \|(\hat{H}(t) - \alpha(t))|\phi(t)\rangle\|, \end{aligned} \quad (4.71)$$

where we use $(\langle\psi(t)| - \langle\phi(t)|)\hat{H}(t)(|\psi(t)\rangle - |\phi(t)\rangle)$ being real in the first equality and the second inequality is a result of the Schwarz inequality. Furthermore, the left hand side of Eq. (4.71) can be represented by

$$\hbar\partial_t\| |\psi(t)\rangle - |\phi(t)\rangle \|^2 = 2\| |\psi(t)\rangle - |\phi(t)\rangle \| \cdot \partial_t\| |\psi(t)\rangle - |\phi(t)\rangle \|. \quad (4.72)$$

Then, eliminating $\| |\psi(t)\rangle - |\phi(t)\rangle \|^2$ from Eqs. (4.71) and (4.72), we get the following inequality

$$\begin{aligned} \hbar\partial_t\| |\psi(t)\rangle - |\phi(t)\rangle \| &\leq \|(\hat{H}(t) - \alpha(t))|\phi(t)\rangle\| \\ &= \|(\hat{H}(t) - \alpha(t))|\psi_0\rangle\|. \end{aligned} \quad (4.73)$$

Integrating both the sides with respect to time, we obtain a fundamental speed limit for the imaginary-time Schrödinger equation as

$$\hbar\| |\psi(\tau)\rangle - e^{-i\int_0^\tau ds\alpha(s)}|\psi_0\rangle \| \leq \int_0^\tau dt\|(\hat{H}(t) - \alpha(t))|\psi_0\rangle\|, \quad (4.74)$$

4.4.2. Speed limit for quantum annealing

Next, we consider the following Hamiltonian for application to quantum annealing,

$$\hat{H}(t) = f(t/\tau)\hat{H}_I + g(t/\tau)\hat{H}_P \quad (4.75)$$

$$|\psi_0\rangle = |G_I\rangle, \quad (4.76)$$

$$\hat{H}_I|G_I\rangle = 0, \quad (4.77)$$

where $0 \leq f(t/\tau), g(t/\tau) \leq 1$, $f(0) = g(1) = 1$, $f(1) = g(0) = 0$, and $|G_I\rangle$ is the ground state of \hat{H}_I . In quantum annealing, the ground state of the initial Hamiltonian \hat{H}_I is trivial and the ground state of the target Hamiltonian \hat{H}_P represents the optimal solution of a combinatorial optimization problem.

We specify the time dependency of $\beta(t)$ as follows,

$$\alpha(t) = \alpha_0 g(t/\tau), \quad (4.78)$$

where α_0 is any time-independent constant. Then, we find that the right hand side of Eq. (4.74) is reduced to

$$\begin{aligned} & \int_0^\tau dt \|(\hat{H}(t) - \alpha(t))|\phi(t)\rangle\| \\ &= \|(\hat{H}_P - \alpha_0)|G_I\rangle\| \left(\int_0^\tau dt g(t/\tau) \right) \\ &= \sqrt{\langle G_I|\hat{H}_P^2|G_I\rangle - \langle G_I|\hat{H}_P|G_I\rangle^2 + (\langle G_I|\hat{H}_P|G_I\rangle - \alpha_0)^2} \\ & \quad \times \left(\int_0^\tau dt g(t/\tau) \right) \\ &\leq \tau \sqrt{\langle G_I|\hat{H}_P^2|G_I\rangle - \langle G_I|\hat{H}_P|G_I\rangle^2 + (\langle G_I|\hat{H}_P|G_I\rangle - \alpha_0)^2}, \end{aligned} \quad (4.79)$$

where we used $0 \leq g(s/\tau) \leq 1$ in the last inequality. Therefore, by setting $\alpha_0 = \langle G_I|\hat{H}_P|G_I\rangle$, we obtain a fundamental speed limit for quantum annealing,

$$\| |\psi(\tau)\rangle - e^{-i\langle G_I|\hat{H}_P|G_I\rangle\tau} |\psi_0\rangle \| \leq \tau \sqrt{\langle G_I|\hat{H}_P^2|G_I\rangle - \langle G_I|\hat{H}_P|G_I\rangle^2}. \quad (4.80)$$

Although this result is general, it is not clear whether Eq. (4.80) is useful for estimating the performance of imaginary-time quantum annealing. Then, in the following, we use Eq. (4.80) to show that the optimal time of the Grover problem in imaginary-time quantum annealing is order $\log N$.

4.4.3. Applicaton to the Grover problem: optimality of

$$\sqrt{M}$$

The Hamiltonian of the Grover problem is given by

$$\hat{H}_I = \mathbf{1} - |g_I\rangle\langle g_I|, \quad (4.81)$$

$$\hat{H}_P = \mathbf{1} - |m\rangle\langle m|. \quad (4.82)$$

In the Grover problem, we start from the ground state of \hat{H}_I , which is $|g_I\rangle$, at initial time $t = 0$, and hope that the state $|\psi(t)\rangle$ reaches the ground state of \hat{H}_P , which is $|m\rangle$, at final time $t = \tau$. The relation between $|g_I\rangle$ and $|m\rangle$ is as follows,

$$\langle g_I|m\rangle = \frac{1}{\sqrt{M}}, \quad (4.83)$$

where M means the size of the problem. We immediately find that the following relations hold,

$$\langle g_I|\hat{H}_P|g_I\rangle = 1 - \frac{1}{M}, \quad (4.84)$$

$$\sqrt{\langle g_I|\hat{H}_P^2|g_I\rangle - \langle g_I|\hat{H}_P|g_I\rangle^2} = \sqrt{\frac{1}{M} - \frac{1}{M^2}}. \quad (4.85)$$

Setting the initial state $|\phi_0\rangle$ to $|g_I\rangle$, we find that Eq. (4.80) is reduced to

$$\| |\psi(\tau)\rangle - e^{-i(1-\frac{1}{M})\int_0^\tau dtg(t/\tau)}|g_I\rangle \| \leq \tau\sqrt{\frac{1}{M} - \frac{1}{M^2}}. \quad (4.86)$$

We consider the case where the state $|\psi(t)\rangle$ reaches the target state $|m\rangle$ at time τ . In the following, we will find the condition that the computational time τ must satisfy. The left hand side of Eq. (4.86) can be evaluated as

$$\begin{aligned} \| |\psi(\tau)\rangle - e^{-i(1-\frac{1}{M})\int_0^\tau dtg(t/\tau)}|g_I\rangle \| &= \| |m\rangle - e^{-i(1-\frac{1}{M})\int_0^\tau dtg(t/\tau)}|g_I\rangle \| \\ &= \left(2 - \frac{2}{\sqrt{M}} \Re e^{-i(1-\frac{1}{M})\int_0^\tau dtg(t/\tau)} \right)^{1/2} \end{aligned} \quad (4.87)$$

Then, from Eqs. (4.86) and (4.87), we find the following inequality

$$\left(2 - \frac{2}{\sqrt{M}} \Re e^{-i(1-\frac{1}{M})\int_0^\tau dtg(t/\tau)} \right)^{1/2} \leq \tau\sqrt{\frac{1}{M} - \frac{1}{M^2}}, \quad (4.88)$$

Therefore, taking the large limit of M , we find

$$\tau \geq \sqrt{2M}, \quad (4.89)$$

which is the necessary condition satisfied by the computational time τ . On the other hand, Ref. [57] finds the explicit schedule which can solve the Grover problem by order \sqrt{M} in quantum annealing. Combining these results, we conclude that the optimal computational time of the Grover problem is of order \sqrt{M} in quantum annealing.

4.5. A useful speed limit for the imaginary-time Schrödinger equation

While we have focused on quantum system so far, QSL is not a purely quantum phenomenon, as shown in Sec. 4.2. In this section, we extend the Kieu bound to the imaginary-time Schrödinger equation. We obtain a fundamental speed limit for the imaginary-time Schrödinger equation which is very similar to the Kieu bound. However, in the imaginary-time Schrödinger equation, the norm of the state is not preserved and it is not clear whether the new bound is tight. Then, we apply it to the Grover problem in imaginary-time quantum annealing. Recent study [111] shows analytically and numerically that the Grover problem in imaginary-time quantum annealing can be solved by order of $\log M$. Here, using our new bound, we show that the optimal computational time is of order $\log M$. This result means that our new bound for the imaginary-time Schrödinger equation is also tight and useful.

4.5.1. Derivation of the speed limit for the imaginary-time Schrödinger equation

We consider two imaginary-time Schrödinger equations and assume that \hat{H} is a real positive-semidefinite matrix and $|\psi(t)\rangle$ and $|\phi(t)\rangle$ are real vectors,

$$-\partial_t|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle, \quad (4.90)$$

$$-\partial_t|\phi(t)\rangle = \beta(t)\mathbf{1}|\phi(t)\rangle, \quad (4.91)$$

$$|\psi(0)\rangle = |\phi(0)\rangle = |\psi_0\rangle, \quad (4.92)$$

where $\beta(t)$ is an arbitrary time-dependent function and $\mathbf{1}$ is the identity matrix. Taking the difference between Eqs. (4.90) and (4.91), we obtain

$$\partial_t(|\psi(t)\rangle - |\phi(t)\rangle) = -\hat{H}(t)(|\psi(t)\rangle - |\phi(t)\rangle) - (\hat{H}(t) - \beta(t))|\phi(t)\rangle. \quad (4.93)$$

Considering the distance between $|\psi(t)\rangle$ and $|\phi(t)\rangle$, we obtain

$$\partial_t \|\psi(t)\rangle - |\phi(t)\rangle\|^2 = 2(\langle\psi(t)| - \langle\phi(t)|)\partial_t(|\psi(t)\rangle - |\phi(t)\rangle). \quad (4.94)$$

Substituting Eq. (4.93) into Eq. (4.94), we obtain

$$\begin{aligned} & \partial_t \|\psi(t)\rangle - |\phi(t)\rangle\|^2 \\ &= -2(\langle\psi(t)| - \langle\phi(t)|)\hat{H}(t)(|\psi(t)\rangle - |\phi(t)\rangle) - 2(\langle\psi(t)| - \langle\phi(t)|)(\hat{H}(t) - \beta(t))|\phi(t)\rangle \\ &\leq -2(\langle\psi(t)| - \langle\phi(t)|)(\hat{H}(t) - \beta(t))|\phi(t)\rangle \\ &\leq 2\|\psi(t)\rangle - |\phi(t)\rangle\| \|(\hat{H}(t) - \beta(t))|\phi(t)\rangle\|, \end{aligned} \quad (4.95)$$

where we used $\hat{H}(t)$ being positive-semidefinite in the first inequality and the second inequality is a result of the Schwarz inequality. Furthermore, the left hand side of Eq. (4.95) can be represented by

$$\partial_t \|\psi(t)\rangle - |\phi(t)\rangle\|^2 = 2\|\psi(t)\rangle - |\phi(t)\rangle\| \partial_t \|\psi(t)\rangle - |\phi(t)\rangle\|. \quad (4.96)$$

Then, eliminating $\|\psi(t)\rangle - |\phi(t)\rangle\|$ from Eqs. (4.95) and (4.96), we get the following inequality

$$\partial_t \|\psi(t)\rangle - |\phi(t)\rangle\| \leq \|(\hat{H}(t) - \beta(t))|\phi(t)\rangle\|. \quad (4.97)$$

Integrating both the sides with respect to time, we obtain a fundamental speed limit for the imaginary-time Schrödinger equation as

$$\|\psi(\tau)\rangle - |\phi(\tau)\rangle\| \leq \int_0^\tau dt \|(\hat{H}(t) - \beta(t))|\phi(t)\rangle\|, \quad (4.98)$$

where $|\phi(t)\rangle = \exp(-\int_0^t ds \beta(s))|\psi_0\rangle$.

Equation (4.98) is the main result of this section which corresponds to Eq. (4.65). However, we note that $|\psi(\tau)\rangle$ and $|\phi(\tau)\rangle$ are not normalized, which is a great difference from the case for quantum system.

4.5.2. Speed limit for time-independent system

First, we consider the time-independent system $\hat{H}(t) = \hat{H}$. We can evaluate the right hand side of Eq. (4.98) as

$$\begin{aligned} \|(\hat{H}(t) - \beta(t))|\phi(t)\rangle\| &= \|(\hat{H} - \beta(t))|\psi_0\rangle\| e^{-\int_0^t ds \beta(s)} \\ &= \sqrt{\langle\psi_0|\hat{H}^2|\psi_0\rangle - \langle\psi_0|\hat{H}|\psi_0\rangle^2 + (\beta(t) - \langle\psi_0|\hat{H}|\psi_0\rangle)^2} \times e^{-\int_0^t ds \beta(s)}. \end{aligned} \quad (4.99)$$

Setting $\beta(t) = \langle \psi_0 | \hat{H} | \psi_0 \rangle$, we obtain

$$\begin{aligned} & \int_0^\tau dt \| (\hat{H}(t) - \beta(t)) | \phi(t) \rangle \| \\ &= \sqrt{\langle \psi_0 | \hat{H}^2 | \psi_0 \rangle - \langle \psi_0 | \hat{H} | \psi_0 \rangle^2} \frac{1 - e^{-\tau \langle \psi_0 | \hat{H} | \psi_0 \rangle}}{\langle \psi_0 | \hat{H} | \psi_0 \rangle}. \end{aligned} \quad (4.100)$$

Therefore, we find that Eq. (4.98) is reduced to

$$\begin{aligned} & \| | \psi(\tau) \rangle - e^{-\tau \langle \psi_0 | \hat{H} | \psi_0 \rangle} | \psi(0) \rangle \| \\ &\leq \sqrt{\langle \psi_0 | \hat{H}^2 | \psi_0 \rangle - \langle \psi_0 | \hat{H} | \psi_0 \rangle^2} \frac{1 - e^{-\tau \langle \psi_0 | \hat{H} | \psi_0 \rangle}}{\langle \psi_0 | \hat{H} | \psi_0 \rangle}. \end{aligned} \quad (4.101)$$

4.5.3. Speed limit for imaginary-time quantum annealing.

Next, we consider the following Hamiltonian for application to imaginary-time quantum annealing,

$$\hat{H}(t) = f(t/\tau) \hat{H}_I + g(t/\tau) \hat{H}_P \quad (4.102)$$

$$| \psi_0 \rangle = | G_I \rangle, \quad (4.103)$$

$$\hat{H}_I | G_I \rangle = 0, \quad (4.104)$$

where $0 \leq f(t/\tau), g(t/\tau) \leq 1$, $f(0) = g(1) = 1$, $f(1) = g(0) = 0$, and $| G_I \rangle$ is the ground state of \hat{H}_I . In quantum annealing, the ground state of the initial Hamiltonian \hat{H}_I is trivial and the ground state of the target Hamiltonian \hat{H}_P represents the optimal solution of a combinatorial optimization problem.

We specify the time dependency of $\beta(t)$ as follows,

$$\beta(t) = \beta_0 g(t/\tau), \quad (4.105)$$

where β_0 is a time-independent any constant. Then, we find that the right hand side of Eq. (4.98) is reduced to

$$\begin{aligned} \int_0^\tau dt \| (\hat{H}(t) - \beta(t)) | \phi(t) \rangle \| &= \| (\hat{H}_P - \beta_0) | G_I \rangle \| \left(\int_0^\tau dt g(t/\tau) e^{-\beta_0 \int_0^t ds g(s/\tau)} \right) \\ &= \sqrt{\langle G_I | \hat{H}_P^2 | G_I \rangle - \langle G_I | \hat{H}_P | G_I \rangle^2 + (\langle G_I | \hat{H}_P | G_I \rangle - \beta_0)^2} \\ &\quad \times \frac{1 - e^{-\beta_0 \int_0^\tau dt g(t/\tau)}}{\beta_0}. \end{aligned} \quad (4.106)$$

Therefore, by setting $\beta_0 = \langle G_I | \hat{H}_P | G_I \rangle$, we obtain a fundamental speed limit for imaginary-time quantum annealing,

$$\begin{aligned} & \| | \psi(\tau) \rangle - e^{-\langle G_I | \hat{H}_P | G_I \rangle \int_0^\tau dt g(t/\tau)} | G_I \rangle \| \\ &\leq \sqrt{\langle G_I | \hat{H}_P^2 | G_I \rangle - \langle G_I | \hat{H}_P | G_I \rangle^2} \frac{1 - e^{-\langle G_I | \hat{H}_P | G_I \rangle \int_0^\tau dt g(t/\tau)}}{\langle G_I | \hat{H}_P | G_I \rangle}. \end{aligned} \quad (4.107)$$

Although this result is general, it is not obvious whether Eq. (4.107) is tight. In the following, to demonstrate that our bound is also useful, we apply Eq. (4.107) to the Grover problem in imaginary-time quantum annealing and show that the optimal computational time is bounded from below by order of $\log M$.

4.5.4. Applicaton to the imaginary-time Grover problem: optimality of $\log M$

The Hamiltonian $\hat{H}(t)$ is a real positive-semidefinite matrix because the eigenvalues are given by

$$0 \leq E_{\pm} = \frac{1}{2} \left(1 \pm \sqrt{1 - 4fg \left(1 - \frac{1}{M} \right)} \right) \leq 1. \quad (4.108)$$

Setting the initial state $|\phi_0\rangle$ to $|g_I\rangle$, we find that Eq. (4.107) is reduced to

$$\| |\psi(\tau)\rangle - e^{-(1-\frac{1}{M}) \int_0^\tau dtg(t/\tau)} |g_I\rangle \| \leq \frac{1 - e^{-\langle g_I | \hat{H}_P | g_I \rangle \int_0^\tau dtg(t/\tau)}}{1 - \frac{1}{M}} \sqrt{\frac{1}{M} - \frac{1}{M^2}}. \quad (4.109)$$

We consider the case where the state $|\psi(t)\rangle$ reaches the target state $\| |\psi(\tau)\rangle \| \cdot |m\rangle$ at time τ . In the following, we will find the condition that the computational time τ must satisfy. The left hand side of Eq. (4.109) can be evaluated as

$$\begin{aligned} & \| |\psi(\tau)\rangle - e^{-(1-\frac{1}{M}) \int_0^\tau dtg(t/\tau)} |g_I\rangle \| \\ &= \| |\psi(\tau)\rangle \| \times |m\rangle - e^{-(1-\frac{1}{M}) \int_0^\tau dtg(t/\tau)} |g_I\rangle \| \\ &= \left(\| |\psi(\tau)\rangle \|^2 + e^{-2(1-\frac{1}{M}) \int_0^\tau dtg(t/\tau)} - \frac{2}{\sqrt{M}} \| |\psi(\tau)\rangle \| e^{-(1-\frac{1}{M}) \int_0^\tau dtg(t/\tau)} \right)^{1/2} \\ &= \left(\left(1 - \frac{1}{M} \right) e^{-2(1-\frac{1}{M}) \int_0^\tau dtg(t/\tau)} + \left(\frac{1}{\sqrt{M}} e^{-(1-\frac{1}{M}) \int_0^\tau dtg(t/\tau)} - \| |\psi(\tau)\rangle \| \right)^2 \right)^{1/2} \\ &\geq \sqrt{\left(1 - \frac{1}{M} \right) e^{-2(1-\frac{1}{M}) \int_0^\tau dtg(t/\tau)}} \\ &\geq \sqrt{\left(1 - \frac{1}{M} \right) e^{-2\tau}}, \end{aligned} \quad (4.110)$$

where we used $0 \leq g(t/\tau) \leq 1$ in the last inequality. Then, from Eqs. (4.109) and (4.110), we find the following inequality

$$\begin{aligned} \sqrt{\left(1 - \frac{1}{M} \right) e^{-2\tau}} &\leq \frac{1 - e^{-\langle g_I | \hat{H}_P | g_I \rangle \int_0^\tau dtg(t/\tau)}}{1 - \frac{1}{M}} \sqrt{\frac{1}{M} - \frac{1}{M^2}} \\ &\leq \frac{1}{1 - \frac{1}{M}} \sqrt{\frac{1}{M} - \frac{1}{M^2}}, \end{aligned} \quad (4.111)$$

where we used also the fact that $0 \leq g(t/\tau) \leq 1$ in the last inequality. Therefore, taking the large limit of M , we find

$$\tau \geq \frac{1}{2} \log(N), \quad (4.112)$$

which is the necessary condition satisfied by the computational time τ . On the other hand, Ref. [111] finds the explicit schedule which can solve the Grover problem by order of $\log M$ in imaginary-time quantum annealing. Combining these results, we conclude that the optimal computational time of the Grover problem is of order $\log M$ in imaginary-time quantum annealing.

Finally, we note that the imaginary-time Grover problem is only a process on a classical computer and it is impossible to physically implement the Grover problem because it is strongly believed that the Grover problem can not be solved earlier than order \sqrt{M} by quantum circuit model.

4.6. Summary

We have provided fundamental speed limits for classical systems. Objects are forbidden from exceeding the speed of light; however, CSL obtained in this chapter is unrelated to the theory of relativity. We have established a trade-off between energy and time in the evolution of classical many-particle systems.

In the classical Liouville equation, the Margolus–Levitin-type bound and the Mandelstam–Tamm-type bound are not independent, and the Mandelstam–Tamm-type bound is always tighter. This is a remarkable difference from the QSL. In addition, since the Liouvillian only contains the first derivative, we can obtain an infinite number of CSLs.

We emphasize that QSL is not based on quantumness. Instead, the QSL is a universal property of dynamical systems described by a Hermitian operator, which enables similar speed limits to be obtained for the imaginary-time Schrödinger equation such as the classical master equation.

It is an interesting problem to investigate whether systems described by the non-Hermitian operator (e.g., the classical master equation not satisfying the detailed balance condition) have fundamental speed limits. Recent studies [128–132] show that a break in the detailed balance condition in the classical master equation accelerates relaxation to the steady state, which suggests that the fundamental speed limit may be essentially changed.

Next, we have extended the Kieu bound to the imaginary-time Schrödinger equation. We applied it to imaginary-time quantum annealing, and showed that

the optimal time of the imaginary-time Grover problem is of order $\log M$, which is consistent with the previous study [111]. This result means that the new bound (4.98) is not only computable but also tight.

In real-time dynamics, the schedule obtained from the adiabatic theorem is optimal [57] and it is possible to prove the optimality of order \sqrt{M} by the fundamental speed limit (4.65). On the other hand, in imaginary-time dynamics, the adiabatic theorem is merely a sufficient condition, and the transition from excited states to the ground state strongly influences and can not be ignored. Thus, the imaginary time adiabatic theorem [51, 133] does not give the optimal schedule [111]. Even in such a case, the fundamental speed limit (4.98) can prove the optimality of order $\log M$. This result means that the adiabatic time evolution has nothing to do with the optimality in imaginary-time dynamics, although the adiabatic time evolution is closely related to the optimality in real-time dynamics. In addition, Ref. [111] pointed out that the imaginary-time annealing is not physically realistic. Our result shows that there is a fundamental limit even in such non-physical systems.

Although we have focused on imaginary-time quantum annealing which corresponds to population annealing [134], it is also expected that the new bound can be applied to estimate the performance of the Fokker-Planck equation. It is a future problem to apply the new bound to other classical algorithms.

5. Conclusion

We have investigated the real and imaginary time dynamical effects of quantum and classical systems, inspired by quantum annealing. In particular, we have examined mean-field quantum spin systems and the quantum speed limit.

Chapter 3 has investigated mean-field quantum spin systems. The main purpose of the chapter is to treat exactly the imaginary-time dependence of the partition function of mean-field quantum spin systems. Mean-field quantum spin systems are one of the simplest quantum spin systems, and there are many studies on them from the view point of quantum annealing. However, mean-field quantum spin systems had been analyzed with the static approximation, which ignores the imaginary-time dependence of the partition function, and had not been solved exactly. In order to solve mean-field quantum spin systems, we have proposed a new method using the optimal control theory. We have mapped a problem of obtaining the exact partition function in the thermodynamic limit to solving the corresponding optimal control problem in the imaginary-time Schrödinger equation. In the optimal control problem, finding the optimal solution is equivalent to solving the corresponding classical Hamilton equations with special initial and terminal conditions. We have applied this identification to a wider class of mean-field quantum spin systems which generalizes the Hopfield model. Although it is very difficult to find an analytical solution of the optimal control problem in general, we can solve the optimal solution and show that the optimal solution coincides with the static approximate solution, that is, the static approximation is exact for a wider class of mean-field quantum spin systems in general. This is a first systematic result for the exactness of the static approximation.

Next, we have applied our result to the previous studies on quantum annealing. We have verified their analysis where the non-stoquastic Hamiltonian [23, 25] and the inhomogeneous transverse field [29] accelerate the computational time exponentially for mean-field quantum spin systems.

Furthermore, we have investigated why our optimal control problem can be solvable because, in general, it is very difficult to solve the optimal control problem exactly [46, 47]. We have examined the corresponding classical Hamiltonian in

detail and, as a result, we have found that the corresponding classical Hamiltonian belongs to classical nonlinear integrable systems. To the best of my knowledge, this classical nonlinear integrable system has not been discovered so far. This means that the new class of classical nonlinear integrable systems is hidden in mean-field quantum spin systems. It is an interesting and urgent problem to obtain further understanding of this classical nonlinear integrable system.

Chapter 4 has generalized the quantum speed limit to classical systems. The main purpose of this chapter is to obtain fundamental speed limits corresponding to the quantum speed limit in classical systems. The quantum speed limit gives an upper bound to the speed of state change of the quantum system and is not only a formal concept but also a useful idea for quantum annealing. Previous studies have regarded the quantum speed limit as a pure quantum phenomenon. On the contrary, we have revealed that classical mechanics also has a similar speed limit. Using the Hilbert space theory for the classical Liouville equation, we have shown that classical mechanics also has fundamental speed limit corresponding to the quantum speed limit. Therefore, the quantum speed limit is not a purely quantum phenomenon but a universal dynamical property of the Hilbert space. In addition, we note that Ref. [135] also finds similar results. Next, we have extended another type of quantum speed limit, which is the Kieu bound, to the imaginary-time Schrödinger equation. In the Grover problem, the Kieu bound is used to prove that the optimal computational time is of order \sqrt{M} in quantum annealing. We have generalized the Kieu bound to the imaginary-time Schrödinger equation and found that the optimal computational time of the Grover problem is bounded below order $\log M$, which is consistent with the previous study [111]. We also note that the imaginary time Schrödinger equation is the dynamics on a classical computer and the physical system corresponding to the imaginary time Grover problem can not exist in real world.

Finally, we mention some related topics in our study. Although we have revealed that the static approximation is exact for a wider class of mean-field quantum spin systems, our method can not analyze systems such as the p -spin-interacting spin glass model with the transverse field where static approximation is not exact [76–84]. In this system, the partition function has a long-range imaginary-time interaction and can not be regarded as the result of the imaginary-time Schrödinger equation. A similar difficulty arises in the Hopfield model with infinite-number patterns in which the static approximation can be broken [85]. It is an extremely important difficult problem to invent a new method for exactly analyzing such systems beyond the static approximation.

In addition, we also mention that the concept of the classical speed limit is recently extended to classical stochastic processes [136, 137]. They found that trade-off inequalities exist between the speed of the state transformation and the entropy production. The concept of the speed limit may further expand.

A. Combinatorial optimization problems

A.1. Combinatorial optimization problems

Let us introduce combinatorial optimization problems. Optimization problems are to optimize the objective under given conditions. A function expressing the efficiency, which depends on problems, is called the cost function and we aim to maximize (or minimize) it. Especially, in the case where the variable is discrete, such a problem is called “combinatorial optimization problems“ [4, 5]. In our daily life, there are many combinatorial optimization problems, for example, searching for train routes, searching for routes of car navigation and scheduling of delivery service. In addition, combinatorial optimization problems are also related to machine learning [138]. In machine learning, we try to express data with a complicated neural network. For this purpose, it is necessary to repeat the adjustment of the parameters included in the neural network, and we optimize the parameters using a large scale computer resource. This is one of the optimization problems. In this way, it is very important to find a better solution of combinatorial optimization problems from a practical point of view.

Let us formulate combinatorial optimization problems. We consider a configuration space of N variables denoted by $\sigma_1, \dots, \sigma_N$, each of which takes discrete values ± 1 . We represent the total configuration as $\sigma = (\sigma_1, \dots, \sigma_N)$. The purpose of combinatorial optimization problems is to find the minimum or maximum of the cost function $E(\sigma)$. We consider only the minimum of $E(\sigma)$ because the maximum of $E(\sigma)$ is equivalent to the minimum of $-E(\sigma)$

The problem is to find an optimal solution which minimizes $E(\sigma)$. However, most of combinatorial optimization problems are too difficult to solve exactly because the size of the configuration space exponentially increases as the size of the problem increases. This is called the combinatorial explosion. Increasing the number of local minima also contributes to making the problem difficult as

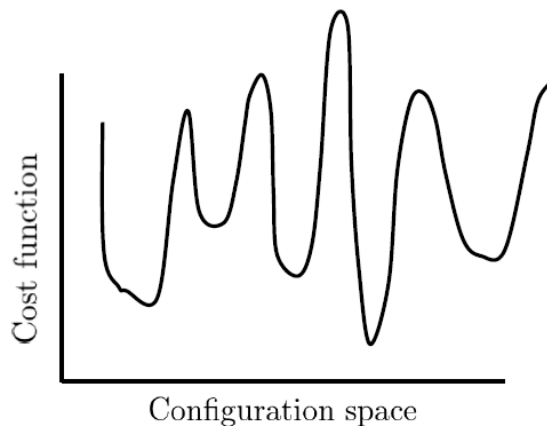


Figure A.1.: A schematic view of the cost function. There are many local minima in the configuration space.

shown in Fig. A.1. In the following section, we introduce a physics approach to combinatorial optimization problems.

A.2. Combinatorial optimization problems and Ising spin systems

Next, we introduce a relation between combinatorial optimization problems and physics. It is known that many combinatorial optimization problems can be translated into physics problems of finding the ground state of Ising spin systems [8–10], for example, the K-SAT problem and the traveling salesman problem. Binary variables and the cost function corresponds to Ising spins and the Hamiltonian of the systems, respectively. The ground state of the Hamiltonian is equivalent to the minimum value of the cost function. For example, we show that the traveling salesman problem, which is one of the combinatorial optimization problems, can be translated into physics problems of finding the ground state of an Ising spin system.

A.2.1. Traveling salesman problem

The traveling salesman problem is as follows [9]. “For given N cities and the path between each pair of cities, what is the best route to pass through all the cities once each and then return?”

First, we denote the distance of the path between city i and city j as d_{ij} . We choose binary units $S_{i,x}$ to represent possible solutions: $S_{i,x} = 1$ means that city i is the x -th stop on the tour and $S_{i,x} = 0$ means anything else. Then, the total length of the path is given by

$$E = \frac{1}{2} \sum_{i,j,x} d_{ij} S_{i,x} (S_{j,x+1} + S_{j,x-1}), \quad (\text{A.1})$$

and there are constraint conditions,

$$\sum_x S_{ix} = 1 \quad (\text{for any city } i), \quad (\text{A.2})$$

$$\sum_i S_{ix} = 1 \quad (\text{for any stop } x). \quad (\text{A.3})$$

The first condition means that each city appears only once on the tour and the second one means that each stop on the tour is at just one city. Therefore, using Eqs. (A.1), (A.2), (A.3), and the transformation $S_{i,x} \rightarrow (\sigma_{i,x} + 1)/2$, we obtain the cost function as follows,

$$H = A \left(\sum_{i,j,x} d_{ij} \sigma_{i,x} (\sigma_{j,x+1} + \sigma_{j,x-1}) + \text{const} \right) + B \left(\sum_x \sigma_{ix} - 1 \right)^2 + C \left(\sum_i \sigma_{ix} - 1 \right)^2 \quad (\text{A.4})$$

where constant terms are omitted and A , B , and C are adjustable parameters. This is the Hamiltonian of an Ising model. In other words, the traveling salesman problem is equivalent to finding the ground state of a spin Hamiltonian. Thus, the traveling salesman problem can be translated into a physics problem of finding the ground state of the spin Hamiltonian.

A.3. Simulated annealing

We have seen that combinatorial optimization problems can be mapped onto classical Ising spin systems. This correspondence allows us to study combinatorial optimization problems using physics ideas. One of the most representative methods is simulated annealing (SA) [11]. This name comes from annealing metalworking. Annealing is a process to optimize the internal structure of metal

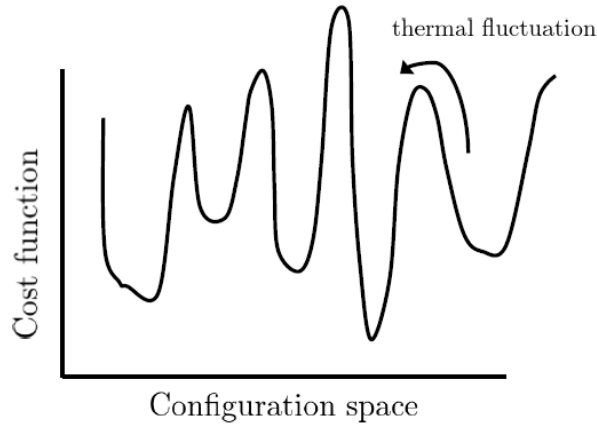


Figure A.2.: A schematic view of simulated annealing. Thermal fluctuations search for an optimal solution

by gradually cooling the molten metal. Eventually, we obtain a stable structure corresponding to the minimum energy state. Simulated annealing introduces temperature T as a global parameter to the Ising spin system which has the ground state corresponding to the optimization problem, and reduces the temperature from a high value to zero. The temperature induces transitions of the state with time evolution stochastically (Markov process). As the transition probability, the Metropolis method is often used,

$$W(E, E') = \begin{cases} 1 & (E - E' \leq 0) \\ \exp(-(E - E')/T) & (E - E' > 0) \end{cases} \quad (\text{A.5})$$

where $W(E, E')$ represents the probability of transition from the state of energy E' to the state of energy E . There are transitions to the high-energy state as well as the low-energy state stochastically. One of the strong points of SA is that it allows the transition to the state with high energy. Thus, it is possible to prevent the state from being trapped in a local minimum and search the configuration space globally. We can understand intuitively that the state can overcome the peaks of potential due to thermal fluctuations as shown in Fig. A.2.

In SA, if we control the system for a sufficiently long time, the state follows the instantaneous equilibrium state and finally reaches the ground state of $T = 0$,

that is, the global minimum. The question is how to control the temperature as a function of time. Of course, the computational time depends on the problem to be considered. However, for an arbitrary cost function, it is known how to change the temperature to obtain the optimal solution with probability 1 in the infinite-time limit. The convergence condition [139] is given by

$$T(t) = \frac{c(N)}{\log(\alpha(N)t + 1)}, \quad (\text{A.6})$$

where $c(N)$ is proportional to N and $\alpha(N)$ is exponentially small in N . If we control the temperature like this, the temperature approaches zero at $t \rightarrow \infty$ and we obtain the optimal solution. From a practical point of view, we need the computational time to be finite and stop the calculation when the temperature becomes sufficiently low. However, when we control the temperature following the above expression, the calculation time diverges exponentially in N because $\alpha(N)$ is exponentially small in N . We note that this is the schedule for most difficult problems and there is also a faster schedule for typical problems.

B. Optimal control theory

In this appendix, we provide some details about the optimal control theory [46,47].

B.1. Optimal control problem

In this section, we provide some knowledge about the optimal control problem.

For m differential equations describing the motion of m dimensional vector $x(s)$,

$$\dot{x}(s) = f(x(s), u(s)), \quad x(0) = x_0, \quad (\text{B.1})$$

let us consider the problem of finding the control input $u(s) \in U(0, T)$ that minimizes the cost function,

$$J = L_f(x(T)) + \int_0^T ds L(x(s), u(s)), \quad (\text{B.2})$$

where the initial state x_0 and the final time T are known and the final state $x(T)$ is arbitrary. Here, using the auxiliary variable k which is the m -dimensional vector, we define the following function,

$$H_{\text{op}} = k^T f(x, u) - L(x, u), \quad (\text{B.3})$$

then, the following result holds.

A necessary condition for the control input $u^*(t)$ and the corresponding trajectory $x^*(t)$ to be optimal is that there exists a function $k^*(t)$ that simultaneously satisfies the following three conditions.

(a) $x^*(t)$ and $k^*(t)$ are solutions to the following ordinary differential equations,

$$\dot{x}^*(s) = \frac{\partial H_{\text{op}}}{\partial k}(x^*(s), u^*(s), k^*(s)), \quad (\text{B.4})$$

$$\dot{k}^*(s) = -\frac{\partial H_{\text{op}}}{\partial x}(x^*(s), u^*(s), k^*(s)). \quad (\text{B.5})$$

(b) $k^*(t)$ satisfies the following boundary condition,

$$k^*(T) = \frac{\partial L_f(x, u)}{\partial x} \Big|_{x=x^*(T)}. \quad (\text{B.6})$$

(c) For any time $s \in [0, T]$,

$$\frac{\partial H_{\text{op}}(x^*(s), u^*(s), k^*(s))}{\partial u^*(s)} = 0. \quad (\text{B.7})$$

B.1.1. Proof

Using the method of Lagrange multiplier, we define the following functional \bar{J} ,

$$\begin{aligned} \bar{J} &= L_f(x(T)) + \int_0^T ds \left\{ L(x(s), u(s)) - k^T(s)(f(x(s), u(s)) - \dot{x}(s)) \right\} \\ &= L_f(x(T)) - \int_0^T ds \left\{ H_{\text{op}}(x(s), u(s)) + k^T(s)\dot{x}(s) \right\}, \end{aligned} \quad (\text{B.8})$$

where k is a Lagrange multiplier. Taking the variation of \bar{J} , we find

$$\begin{aligned} \delta \bar{J} &= \frac{\partial L_f(x(T))}{\partial x} \delta x(T) - \int_0^T \left(\frac{\partial H_{\text{op}}}{\partial x} \delta x + \frac{\partial H_{\text{op}}}{\partial u} \delta u - k^T \delta \dot{x} \right) ds \\ &= \frac{\partial L_f(x(T))}{\partial x} \delta x(T) - [k^T \delta x]_0^T - \int_0^T \left(\frac{\partial H_{\text{op}}}{\partial x} \delta x + \frac{\partial H_{\text{op}}}{\partial u} \delta u + \dot{k}^T \delta x \right) ds \\ &= \left(\frac{\partial L_f(x(T))}{\partial x} - k^T(T) \right) \delta x(T) - \int_0^T \left\{ \left(\frac{\partial H_{\text{op}}}{\partial x} + \dot{k}^T \right) \delta x + \frac{\partial H_{\text{op}}}{\partial u} \delta u \right\} ds, \end{aligned} \quad (\text{B.9})$$

where we used $\delta x(0) = 0$ because $x(0) = x_0$ is fixed. Thus, when \bar{J} is optimal, we obtain Eqs. (B.3), (B.4), (B.5), (B.6) and (B.7).

B.1.2. Application to infinite-range ferromagnetic p -spin model

From the imaginary-time Schrödinger equation (3.34), we obtain

$$\dot{x}_1(s) = p(m^z(s))^{p-1}x_1(s) - (p-1)(m^z(s))^p x_1(s) + \Gamma x_2(s) = f_1(x(s), m^z(s)), \quad (\text{B.10})$$

$$\dot{x}_2(s) = \Gamma x_1(s) - p(m^z(s))^{p-1}x_2(s) - (p-1)(m^z(s))^p x_2(s) = f_2(x(s), m^z(s)), \quad (\text{B.11})$$

$$\dot{x}_3(s) = p(m^z(s))^{p-1}x_3(s) - (p-1)(m^z(s))^p x_3(s) + \Gamma x_4(s) = f_3(x(s), m^z(s)), \quad (\text{B.12})$$

$$\dot{x}_4(s) = \Gamma x_3(s) - p(m^z(s))^{p-1}x_4(s) - (p-1)(m^z(s))^p x_4(s) = f_4(x(s), m^z(s)), \quad (\text{B.13})$$

$$x_1(0) = x_4(0) = 1, \quad x_2(0) = x_3(0) = 0, \quad (\text{B.14})$$

and the cost function is given by

$$L_f(x(\beta)) = -x_1(\beta) - x_4(\beta), \quad (\text{B.15})$$

$$L = 0. \quad (\text{B.16})$$

Therefore, we arrive at the corresponding classical Hamiltonian

$$H_{\text{op}} = -(p-1)(m^z)^p \sum_{i=1}^4 x_i k_i + p(m^z)^{p-1} \sum_{i=1}^4 (-1)^{i-1} x_i k_i, \quad (\text{B.17})$$

and the initial and terminal conditions

$$x_1(0) = x_4(0) = 1, \quad x_2(0) = x_3(0) = 0, \quad (\text{B.18})$$

$$k_1(\beta) = k_4(\beta) = -1, \quad k_2(\beta) = k_3(\beta) = 0. \quad (\text{B.19})$$

B.1.3. Application to generalized Hopfield model

From the imaginary-time Schrödinger equation (3.72), we obtain

$$\begin{aligned}
& \dot{x}_{4i-3}(s) \\
= & \sum_{\mu} J_i^{\mu} f'_{\mu}(m_{\mu}^z(t)) x_{4i-3}(s) + \sum_{\nu} \Gamma_i^{\nu} g'_{\nu}(m_{\nu}^x(t)) x_{4i-2}(s) \\
& + \left\{ \sum_{\mu} \left(-f'_{\mu}(m_{\mu}^z(t)) \cdot m_{\mu}^z(t) + f_{\mu}(m_{\mu}^z(t)) \right) + \sum_{\nu} \left(-g'_{\nu}(m_{\nu}^x(t)) \cdot m_{\nu}^x(t) + g_{\nu}(m_{\nu}^x(t)) \right) \right\} x_{4i-3}(s) \\
= & f_{4i-3}(x(s), m^z(s)) \tag{B.20}
\end{aligned}$$

$$\begin{aligned}
& \dot{x}_{4i-2}(s) \\
= & \sum_{\nu} \Gamma_i^{\nu} g'_{\nu}(m_{\nu}^x(t)) x_{4i-3}(s) - \sum_{\mu} J_i^{\mu} f'_{\mu}(m_{\mu}^z(t)) x_{4i-2}(s) \\
& + \left\{ \sum_{\mu} \left(-f'_{\mu}(m_{\mu}^z(t)) \cdot m_{\mu}^z(t) + f_{\mu}(m_{\mu}^z(t)) \right) + \sum_{\nu} \left(-g'_{\nu}(m_{\nu}^x(t)) \cdot m_{\nu}^x(t) + g_{\nu}(m_{\nu}^x(t)) \right) \right\} x_{4i-2}(s) \\
= & f_{4i-2}(x(s), m^z(s)) \tag{B.21}
\end{aligned}$$

$$\begin{aligned}
& \dot{x}_{4i-1}(s) \\
= & \sum_{\mu} J_i^{\mu} f'_{\mu}(m_{\mu}^z(t)) x_{4i-1}(s) + \sum_{\nu} \Gamma_i^{\nu} g'_{\nu}(m_{\nu}^x(t)) x_{4i}(s) \\
& + \left\{ \sum_{\mu} \left(-f'_{\mu}(m_{\mu}^z(t)) \cdot m_{\mu}^z(t) + f_{\mu}(m_{\mu}^z(t)) \right) + \sum_{\nu} \left(-g'_{\nu}(m_{\nu}^x(t)) \cdot m_{\nu}^x(t) + g_{\nu}(m_{\nu}^x(t)) \right) \right\} x_{4i-1}(s) \\
= & f_{4i-1}(x(s), m^z(s)) \tag{B.22}
\end{aligned}$$

$$\begin{aligned}
& \dot{x}_{4i}(s) \\
= & \sum_{\nu} \Gamma_i^{\nu} g'_{\nu}(m_{\nu}^x(t)) x_{4i-1}(s) - \sum_{\mu} J_i^{\mu} f'_{\mu}(m_{\mu}^z(t)) x_{4i}(s) \\
& + \left\{ \sum_{\mu} \left(-f'_{\mu}(m_{\mu}^z(t)) \cdot m_{\mu}^z(t) + f_{\mu}(m_{\mu}^z(t)) \right) + \sum_{\nu} \left(-g'_{\nu}(m_{\nu}^x(t)) \cdot m_{\nu}^x(t) + g_{\nu}(m_{\nu}^x(t)) \right) \right\} x_{4i}(s) \\
= & f_{4i}(x(s), m^z(s)) \tag{B.23}
\end{aligned}$$

$$x_{4j-3}(0) = x_{4j}(0) = 1, \tag{B.24}$$

$$x_{4j-2}(0) = x_{4j-1}(0) = 0, \tag{B.25}$$

and

$$L_f(x(\beta)) = - \prod_i^N (x_{4i-3}(\beta) + x_{4i}(\beta)) \tag{B.26}$$

$$L = 0 \tag{B.27}$$

Then, from the optimal control theory, we obtain the classical Hamiltonian

$$\begin{aligned}
H_{\text{op}}(x, k, m_{\mu}^z, m_{\nu}^x) &= \left\{ \sum_{\mu} \left(-f'_{\mu}(m_{\mu}^z) m_{\mu}^z + f_{\mu}(m_{\mu}^z) \right) + \sum_{\nu} \left(-g'_{\nu}(m_{\nu}^x) m_{\nu}^x + g_{\nu}(m_{\nu}^x) \right) \right\} \sum_{i=1}^{4N} x_i k_i \\
&+ \sum_{\mu} \sum_{i=1}^N J_i^{\mu} f'_{\mu}(m_{\mu}^z) (x_{4i-3} k_{4i-3} - x_{4i-2} k_{4i-2} + x_{4i-1} k_{4i-1} - x_{4i} k_{4i}) \\
&+ \sum_{\nu} \sum_{i=1}^N \Gamma_i^{\nu} g'_{\nu}(m_{\nu}^x) (x_{4i-3} k_{4i-2} + x_{4i-2} k_{4i-3} + x_{4i-1} k_{4i} + x_{4i} k_{4i-1}),
\end{aligned} \tag{B.28}$$

and the boundary conditions

$$k_{4j-3}(\beta) = k_{4j}(\beta) = - \prod_{i=1, i \neq j}^N (x_{4i-3}(\beta) + x_{4i}(\beta)), \tag{B.29}$$

$$k_{4j-2}(\beta) = k_{4j-1}(\beta) = 0. \tag{B.30}$$

C. Derivation of the partition function with imaginary-time dependence

In this chapter, we provide the details on the derivation of the partition function.

C.1. Generalized Hopfield model

We consider the generalized Hopfield model,

$$\hat{H}_G = -N \sum_{\mu=1}^k f_{\mu} \left(\frac{1}{N} \sum_{i=1}^N J_i^{\mu} \hat{\sigma}_i^z \right) - N \sum_{\nu=1}^l g_{\nu} \left(\frac{1}{N} \sum_{i=1}^N \Gamma_i^{\nu} \hat{\sigma}_i^x \right). \quad (\text{C.1})$$

where f_{μ} and g_{ν} are arbitrary functions and J_i^{μ} and Γ_i^{ν} depend on site i .

The difference from the p -spin model with the transverse field is to introduce the order parameters in the x direction. In addition, it is also necessary to introduce the order parameters as many as the number of patterns. Using the Suzuki-Trotter decomposition and the closure relation

$$\hat{1} = \sum_{\{\sigma_i^z(t)=\pm 1\}} |\{\sigma_i^z(t)\}\rangle \langle \{\sigma_i^z(t)\}| \sum_{\{\sigma_i^x(t)=\pm 1\}} |\{\sigma_i^x(t)\}\rangle \langle \{\sigma_i^x(t)\}| \quad (\text{C.2})$$

We arrive at

$$\begin{aligned} Z &= \text{Tr} e^{-\beta \hat{H}_G} \\ &= \lim_{M \rightarrow \infty} \prod_{t=1}^M \sum_{\{\sigma_i^z(t)=\pm 1\}} \sum_{\{\sigma_i^x(t)=\pm 1\}} \langle \{\sigma_i^z(t)\} | e^{\frac{\beta N}{M} \sum_{\mu=1}^k f_{\mu} \left(\frac{1}{N} \sum_{i=1}^N J_i^{\mu} \sigma_i^z(t) \right)} | \{\sigma_i^x(t)\} \rangle \\ &\quad \langle \{\sigma_i^x(t)\} | e^{\frac{\beta N}{M} \sum_{\nu=1}^l g_{\nu} \left(\frac{1}{N} \sum_{i=1}^N \Gamma_i^{\nu} \sigma_i^x(t) \right)} | \{\sigma_i^z(t+1)\} \rangle, \end{aligned} \quad (\text{C.3})$$

where $\{\sigma_i^x = \pm 1\}$ represents the sum of the x bases for all spins and $|\{\sigma_i^x\}\rangle$ describes the orthonormal basis that diagonalizes the x -component of the Pauli matrices.

Using the Dirac delta function and its Fourier representation,

$$e^{\frac{\beta N}{M} f_\mu(\frac{1}{N} \sum_{i=1}^N J_i^\mu \sigma_i^z(t))} = \int dm_\mu^z(t) \int d\tilde{m}_\mu^z(t) e^{\beta N f_\mu(m_\mu^z(t))/M} e^{-N \tilde{m}_\mu^z(t)(m_\mu^z(t) - \frac{1}{N} \sum_{i=1}^N J_i^\mu \sigma_i^z(t))}, \quad (\text{C.4})$$

$$e^{\frac{\beta N}{M} g_\nu(\frac{1}{N} \sum_{i=1}^N \Gamma_i^\nu \sigma_i^x(t))} = \int dm_\nu^x(t) \int d\tilde{m}_\nu^x(t) e^{\beta N g_\nu(m_\nu^x(t))/M} e^{-N \tilde{m}_\nu^x(t)(m_\nu^x(t) - \frac{1}{N} \sum_{i=1}^N \Gamma_i^\nu \sigma_i^x(t))}, \quad (\text{C.5})$$

we can represent the partition function as

$$\begin{aligned} Z &= \text{Tr} e^{-\beta \hat{H}_G} \\ &= \lim_{M \rightarrow \infty} \prod_{t=1}^M \sum_{\{\sigma_i^z(t)=\pm 1\}} \sum_{\{\sigma_i^x(t)=\pm 1\}} \left(\prod_{\mu, \nu} \int dm_\mu^z(t) \int d\tilde{m}_\mu^z(t) \int dm_\nu^x(t) \int d\tilde{m}_\nu^x(t) \right) \\ &\quad e^{\sum_\mu (\beta N f_\mu(m_\mu^z(t))/M - N \tilde{m}_\mu^z(t) m_\mu^z(t)) + \sum_\nu (\beta N g_\nu(m_\nu^x(t))/M - N \tilde{m}_\nu^x(t) m_\nu^x(t))} \\ &\quad \langle \{\sigma_i^z(t)\} | e^{\sum_\mu \tilde{m}_\mu^z(t) \sum_{i=1}^N J_i^\mu \sigma_i^z(t)} | \{\sigma_i^x(t)\} \rangle \langle \{\sigma_i^x(t)\} | e^{\sum_\nu \tilde{m}_\nu^x(t) \sum_{i=1}^N \Gamma_i^\nu \sigma_i^x(t)} | \{\sigma_i^z(t+1)\} \rangle, \end{aligned} \quad (\text{C.6})$$

Furthermore, using the closure relation and the saddle point equation,

$$\tilde{m}_\mu^z(t) = \frac{\beta}{M} f'(m_\mu^z(t)) \quad (\text{C.7})$$

$$\tilde{m}_\nu^x(t) = \frac{\beta}{M} g'(m_\nu^x(t)) \quad (\text{C.8})$$

we obtain the partition function of the Generalized Hopfield model

$$\begin{aligned} Z &= \lim_{M \rightarrow \infty} \left(\prod_{t=1}^M \prod_{\mu, \nu} \int dm_\mu^z(t) \int dm_\nu^x(t) \right) \prod_{i=1}^N \left\{ \text{Tr} \left(\prod_{t=1}^M e^{\frac{\beta}{M} \sum_\mu J_i^\mu f'_\mu(m_\mu^z(t)) \hat{\sigma}^z} e^{\frac{\beta}{M} \sum_\nu \Gamma_i^\nu g'_\nu(m_\nu^x(t)) \hat{\sigma}^x} \right. \right. \\ &\quad \left. \left. e^{\frac{\beta}{M} \left\{ \sum_\mu (-f'_\mu(m_\mu^z(t)) \cdot m_\mu^z(t) + f_\mu(m_\mu^z(t))) + \sum_\nu (-g'_\nu(m_\nu^x(t)) \cdot m_\nu^x(t) + g_\nu(m_\nu^x(t))) \right\}} \right) \right\}. \end{aligned} \quad (\text{C.9})$$

C.2. Further generalization

Next, we consider a more general case,

$$\hat{H} = -N \sum_\mu f_\mu \left(\frac{1}{N} \hat{H}_{1,\mu}(\{\hat{\sigma}^z\}) \right) - N \sum_\nu g_\nu \left(\frac{1}{N} \hat{H}_{2,\nu}(\{\hat{\sigma}^x\}) \right), \quad (\text{C.10})$$

where f_μ and g_ν are arbitrary functions, $\hat{H}_{1,\mu}(\{\hat{\sigma}^z\})$ and $\hat{H}_{2,\nu}(\{\hat{\sigma}^x\})$ are arbitrary Hamiltonians composed of $\{\hat{\sigma}^z\}$ and $\{\hat{\sigma}^x\}$, respectively. We assume that their

eigenvalues are proportional to the system size N in order to satisfy the extensive property.

There is no difference from the generalized Hopfield model. Using the Suzuki-Trotter decomposition and the closure relation, we arrive at

$$\begin{aligned}
Z &= \lim_{M \rightarrow \infty} \prod_{t=1}^M \sum_{\{\sigma_i^z(t)=\pm 1\}} \sum_{\{\sigma_i^x(t)=\pm 1\}} \langle \{\sigma_i^z(t)\} | e^{\frac{\beta N}{M} \sum_{\mu=1}^k f_{\mu}(\frac{1}{N} H_{1,\mu}(\{\sigma^z\}))} | \{\sigma_i^x(t)\} \rangle \\
&\quad \langle \{\sigma_i^x(t)\} | e^{\frac{\beta N}{M} \sum_{\nu=1}^l g_{\nu}(\frac{1}{N} H_{2,\nu}(\{\sigma^x\}))} | \{\sigma_i^z(t+1)\} \rangle, \tag{C.11}
\end{aligned}$$

From the Dirac delta function and its Fourier representation,

$$\begin{aligned}
&e^{\frac{\beta N}{M} f_{\mu}(\frac{1}{N} H_{1,\mu}(\{\sigma^z\}))} \\
&= \int dm_{\mu}^z(t) \int d\tilde{m}_{\mu}^z(t) e^{\beta N f_{\mu}(m_{\mu}^z(t))/M} e^{-N \tilde{m}_{\mu}^z(t)(m_{\mu}^z(t) - \frac{1}{N} H_{1,\mu}(\{\sigma^z\}))}, \tag{C.12}
\end{aligned}$$

$$\begin{aligned}
&e^{\frac{\beta N}{M} g_{\nu}(\frac{1}{N} H_{2,\nu}(\{\sigma^x\}))} \\
&= \int dm_{\nu}^x(t) \int d\tilde{m}_{\nu}^x(t) e^{\beta N g_{\nu}(m_{\nu}^x(t))/M} e^{-N \tilde{m}_{\nu}^x(t)(m_{\nu}^x(t) - \frac{1}{N} H_{2,\nu}(\{\sigma^x\}))}, \tag{C.13}
\end{aligned}$$

the partition function is given by

$$\begin{aligned}
Z &= \left(\prod_{t=1}^M \prod_{\mu,\nu} \int dm_{\mu}^z(t) \int dm_{\nu}^x(t) \right) \text{Tr} \left(\prod_{t=1}^M e^{\frac{\beta}{M} \sum_{\mu} f'_{\mu}(m_{\mu}^z(t)) \hat{H}_{1,\mu}(\{\hat{\sigma}^z\})} e^{\frac{\beta}{M} \sum_{\nu} g'_{\nu}(m_{\nu}^x(t)) \hat{H}_{2,\nu}(\{\hat{\sigma}^x\})} \right. \\
&\quad \left. e^{\left[\frac{N\beta}{M} \left\{ -\sum_{\mu} f'_{\mu}(m_{\mu}^z(t)) \cdot m_{\mu}^z(t) + \sum_{\mu} f_{\mu}(m_{\mu}^z(t)) - \sum_{\nu} g'_{\nu}(m_{\nu}^x(t)) \cdot m_{\nu}^x(t) + \sum_{\nu} g_{\nu}(m_{\nu}^x(t)) \right\} \right]} \right). \tag{C.14}
\end{aligned}$$

D. Hilbert space for Classical Liouville equation

In this appendix, we provide some details about the Hilbert space for the classical Liouville equation.

D.1. Liouvillian as a Hermitian operator

We show that the Liouvillian is a Hermitian operator. For simplicity, we consider a one-dimensional system. We obtain

$$\begin{aligned}
\langle \rho_1(t) | (\hat{L} | \rho_2(t') \rangle) &\equiv \int \int dx dp \rho_1^*(x, p, t) (\hat{L} \rho_2(x, p, t)) \\
&= i \int \int dx dp \rho_1^*(x, p, t) \{H, \rho_2(x, p, t)\} \\
&= i \int \int dx dp \left(\rho_1^*(x, p, t) \frac{\partial H(x, p)}{\partial x} \frac{\partial \rho_2(x, p, t)}{\partial p} \right. \\
&\quad \left. - \rho_1^*(x, p, t) \frac{\partial H(x, p)}{\partial p} \frac{\partial \rho_2(x, p, t)}{\partial x} \right) \\
&= i \int \int dx dp \left(-\frac{\partial \rho_1^*(x, p, t)}{\partial p} \frac{\partial H(x, p)}{\partial x} \rho_2(x, p, t) \right. \\
&\quad \left. + \frac{\partial \rho_1^*(x, p, t)}{\partial x} \frac{\partial H(x, p)}{\partial p} \rho_2(x, p, t) \right) \\
&= -i \int \int dx dp \{H, \rho_1^*(x, p, t)\} \rho_2(x, p, t) \\
&= \int \int dx dp (\hat{L} \rho_1(x, p, t))^* \rho_2(x, p, t) \\
&= (\langle \rho_1(t) | \hat{L} | \rho_2(t') \rangle), \tag{D.1}
\end{aligned}$$

where we used the fact that the surface term vanishes. Therefore, the Liouvillian \hat{L} is a Hermitian operator.

D.2. Proof of $\langle \rho(t) | \hat{L} | \rho(t) \rangle = 0$

We evaluate $\langle \rho(t) | \hat{L} | \rho(t) \rangle$ as

$$\begin{aligned}
\langle \rho(t) | \hat{L} | \rho(t) \rangle &= i \int \int dx dp \left(\rho^*(x, p, t) \frac{\partial H(x, p)}{\partial x} \frac{\partial \rho(x, p, t)}{\partial p} - \rho^*(x, p, t) \frac{\partial H(x, p)}{\partial p} \frac{\partial \rho(x, p, t)}{\partial x} \right) \\
&= i \int \int dx dp \left(-\frac{\partial \rho^*(x, p, t)}{\partial x} H(x, p) \frac{\partial \rho(x, p, t)}{\partial p} - \rho^*(x, p, t) H(x, p) \frac{\partial \rho(x, p, t)}{\partial x \partial p} \right. \\
&\quad \left. + \frac{\partial \rho^*(x, p, t)}{\partial p} H(x, p) \frac{\partial \rho(x, p, t)}{\partial x} + \rho^*(x, p, t) H(x, p) \frac{\partial \rho(x, p, t)}{\partial p \partial x} \right) \\
&= i \int \int dx dp H(x, p) \{ \rho(x, p, t), \rho^*(x, p, t) \}, \tag{D.2}
\end{aligned}$$

where we used the fact that the surface term vanishes. Then, if $\rho(x, p, t)$ is a real-valued function, we obtain

$$\langle \rho(t) | \hat{L} | \rho(t) \rangle = \sum_n |c_n|^2 \lambda_n = 0. \tag{D.3}$$

D.3. Eigenvalues of the Liouvillian

The eigenvalue equation of the Liouvillian is given by

$$\begin{aligned}
\hat{L} \rho_n(x, p) &= i \frac{\partial H(x, p)}{\partial x} \frac{\partial \rho_n(x, p)}{\partial p} - i \frac{\partial H(x, p)}{\partial p} \frac{\partial \rho_n(x, p)}{\partial x} \\
&= \left(-\frac{\partial H(x, p)}{\partial x} \frac{\partial g_n(x, p)}{\partial p} + \frac{\partial H(x, p)}{\partial p} \frac{\partial g_n(x, p)}{\partial x} \right) \\
&\quad + i \left(\frac{\partial H(x, p)}{\partial x} \frac{\partial f_n(x, p)}{\partial p} - \frac{\partial H(x, p)}{\partial p} \frac{\partial f_n(x, p)}{\partial x} \right) \\
&= \lambda_n (f_n(x, p) + i g_n(x, p)), \tag{D.4}
\end{aligned}$$

where

$$\rho_n(x, p) = f_n(x, p) + i g_n(x, p) \tag{D.5}$$

is the eigenfunction. From the above equations, we immediately find that the complex conjugate of $\rho_n(x, p)$ satisfies

$$\hat{L} \rho_n^*(x, p) = -\lambda_n \rho_n^*(x, p). \tag{D.6}$$

Therefore, if λ_n is an eigenvalue of the Liouvillian, $-\lambda_n$ is also an eigenvalue of the Liouvillian.

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List of Publicatios

Publications on which this thesis is built

- [1] M. Okuyama and M. Ohzeki, Quantum speed limit is not quantum, *Phys. Rev. Lett.* **120**, 070402 (2018),
- [2] M. Okuyama and M. Ohzeki, A useful fundamental speed limit for the imaginary-time Schrodinger equation, arXiv:1806.09040 (2018),
- [3] M. Okuyama and M. Ohzeki, An exact solution of the partition function for mean-field quantum spin systems without the static approximation, arXiv:1808.09707 (2018),

Other publications

- [1] M. Okuyama, Y. Yamanaka, H. Nishimori and M. M. Rams, Anomalous behavior of the energy gap in the one-dimensional quantum XY model, *Phys. Rev. E* **92**, 052116 (2015).
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