Statistical ensembles for phase coexistence states specified by noncommutative additive observables

Yasushi Yoneta\textsuperscript{1,2,*} and Akira Shimizu\textsuperscript{3,2†}

\textsuperscript{1}Department of Basic Science, The University of Tokyo, 3-8-1 Komaba, Meguro, Tokyo 153-8902, Japan
\textsuperscript{2}RIKEN Center for Quantum Computing, 2-1 Hirosawa, Wako City, Saitama 351-0198, Japan
\textsuperscript{3}Institute for Photon Science and Technology, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan

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A phase coexistence state cannot be specified uniquely by any intensive parameters, such as the temperature and the magnetic field, because they take the same values over all coexisting phases. It can be specified uniquely only by an appropriate set of additive observables. Hence, to analyze phase coexistence states the statistical ensembles that are specified by additive observables have been employed, such as the microcanonical and restricted ensembles. However, such ensembles are ill-defined or ill-behaved when some of the additive observables do not commute with each other. Here, we solve this fundamental problem by extending a generalized ensemble in such a way that it is applicable to phase coexistence states which are specified by noncommutative additive observables.

We prove that this ensemble correctly gives the density matrix corresponding to phase coexistence states of general quantum systems as well as the thermodynamic functions. Furthermore, these ensembles are convenient for practical calculations because of their good analytic properties and useful formulas by which temperature and other intensive parameters are directly obtained from the expectation values of the additive observables. As a demonstration, we apply our formulation to a two-dimensional system whose phase coexistence states are specified by an additive observable (order parameter) that does not commute with the Hamiltonian.

I. INTRODUCTION

Phase coexistence states are widely observed in nature and have long been attracting much attention. For example, the interfaces separating the coexisting phases, called 'phase interfaces' or 'domain walls', play key roles in various fields of science, such as surface physics, soft matter physics, chemistry, and biology \cite{1,2}. Phase coexistence states also attract a lot of attention from a viewpoint of engineering because the phase interfaces can possess exotic properties that are absent in the bulk, such as multifacility, superconductivity, and semiconductivity \cite{3}. For instance, there is a growing movement to realize next-generation devices utilizing such functional properties of phase interfaces \cite{6,9}.

Recently, the use of quantum fluctuations has been proposed to control the phase interface at low temperatures, where thermal fluctuations are negligible, and the experiment has been conducted \cite{10}. However, it is a challenging task with current technology to observe the microscopic structure of the phase interface because the experiments are performed under extreme conditions. Therefore, it is important to theoretically analyze quantum systems that exhibit phase coexistence.

However, phase coexistence states are particularly difficult to study theoretically because they are related to first-order phase transitions where the thermodynamic properties have particularly strong singularities. In fact, there has been no concrete method that can be systematically applied to phase coexistence states of general quantum systems for the following reason.

In statistical mechanics, statistical ensembles play a fundamental role \cite{1,10,11,13}, and various types of ensembles have been devised \cite{14,29}. The thermodynamic functions of the macroscopic systems with short-range interactions are independent of the ensemble used in the calculation \cite{30}. This fact is called the 'equivalence of ensembles'. Therefore, to obtain thermodynamic functions of the macroscopic system, one can employ any ensemble. However, to investigate other properties, such as microscopic structures of the phase interfaces or thermodynamics of the systems with finite-size effects, one must choose an appropriate ensemble.

The appropriate choice of the ensemble is particularly important in the first-order phase transition region, where several phases can coexist in various proportions \cite{31,32}. The coexisting phases in a phase coexistence state cannot be distinguished by any intensive parameters, such as the temperature and the magnetic field, because every intensive parameter takes the same value between the coexisting phases. For this reason, the canonical ensemble (CE) that specified by intensive parameters can give only particular states among the various states in the first-order phase transition region.

For example, when the periodic boundary conditions are imposed, the CE gives either a single-phase state or a statistical mixture of single-phase states, and it cannot give a phase coexistence state (see Refs. \cite{29,33}; we will also give examples in Section \textsuperscript{X}). This problem of the CE can be solved for some specific models by imposing clever boundary conditions \cite{34,36}. However, for general
systems such as systems with a disordered phase, it is not clear whether such boundary conditions exist and what boundary conditions should be imposed.

The coexisting phases in a phase coexistence state can be distinguished not by an intensive parameter but by a proper additive quantity, called the ‘order parameter’ (in a broad sense). Therefore, the microcanonical ensemble (MCE) can give phase coexistence states for general systems because it is specified by a set of additive quantities including the order parameter. This makes it possible to investigate microscopic structures, such as those of phase interfaces, of the phase coexistence state [37].

The characteristics of different ensembles are also pronounced when investigating finite systems because the equivalence of ensembles does not hold for finite systems [33, 37, 38]. For example, in finite systems which undergo first-order phase transitions in the thermodynamic limit (TDL), the concavity of the microcanonical entropy is broken generally, even with short-range interactions (see Appendix C of Ref. [29]). This concavity breaking leads to thermodynamic anomalies such as the negative specific heat [33, 39–45], which was indeed observed experimentally [46–48]. Nevertheless, the CE fails to give such thermodynamic anomalies of finite systems, while the MCE correctly gives them directly and quantitatively [26, 33, 37, 38, 49–53].

Unfortunately, however, the MCE has a fundamental problem in quantum systems when the additive observables that specify the MCE do not commute with each other. Since such observables cannot be diagonalized simultaneously, it is generally impossible to construct the MCE using their simultaneous eigenstates. A similar problem is also present in the restricted ensemble (RE), which is obtained by projecting the CE onto the subspace spanned by the eigenstates of an additive observable [20, 27, 54]. Such a projection often generates a superposition of macroscopically distinct states [55], which cannot be a thermal equilibrium state. (See Section III for these problems of the MCE and the RE.)

To resolve the problem of noncommutative additive observables, von Neumann proposed constructing the MCE using a commutative set of observables that approximate the original set of additive observables [57]. However, such a set of commutative observables are hard to construct, and their explicit forms are obtained only in limited cases [55, 51]. That is, so far, no method has been established for constructing the MCE or any other ensembles for the noncommutative additive observables for general quantum systems.

In this paper, we solve this fundamental problem by extending a generalized ensemble in such a way that it can be applied to phase coexistence states which are specified by noncommutative additive observables. Among various generalized ensembles, we focus on the squeezed ensemble (SE) [29], which is a particularly broad class of statistical ensembles. Originally, the SE was introduced for systems whose equilibrium states can be specified uniquely only by the internal energy and the number of spins. We extend the SE so that it can be defined for systems whose equilibrium states are specified by three or more additive observables which can be noncommutative.

For this ensemble, we prove that all the additive observables have macroscopically definite values even when they do not commute with each other. Therefore, by using the SE, one can correctly obtain the desired phase coexistence states of general quantum systems without any ad hoc procedures, such as devising boundary conditions.

In addition, we derive useful formulas for thermodynamic quantities, such as the thermodynamic entropy and the intensive parameters. The intensive parameters can be calculated efficiently by the formulas, without resorting to numerical differentiation of the thermodynamic function. Therefore, by using the SE, one can fully investigate the thermodynamic properties of the equilibrium states.

This paper is organized as follows. In Section II, we describe the setup and notation. In Section III, we review the difficulties faced by conventional ensembles which have been employed to study phase coexistence states, due to the noncommutativity of additive observables. In Section IV, we define the SE for quantum systems whose equilibrium states are specified by noncommutative additive observables. In Sections V and VI, we investigate the basic properties of the SE. We show that the SE always gives the correct equilibrium state. In addition, we derive formulas for the thermodynamic entropy density and intensive parameters. First, in Section V, we consider the case where the additive observables commute with each other. Next, in Section VI, we consider the noncommutative case. In Section VII, we discuss the parameter dependence of the SE. In Section VIII, we summarize the usage of the SE. In Section IX, we apply our formulation to the free spins and demonstrate its validity. In Section X, we apply our formulation to the two-dimensional transverse field Ising model, which has coexisting phases distinguished by the order parameter which does not commute with the Hamiltonian, and demonstrate that the SE successfully gives phase coexistence states even in such a case which cannot be treated by conventional ensembles. In Section XI, we provide our conclusions and discussion.

II. SETUP AND NOTATION

In this section, we describe the setup and notation of our formulation.

A. Setup

We consider a sequence, indexed by the number of lattice sites $N$, of quantum spin systems on the hypercubic lattice with short-range interactions. We assume that the equilibrium state for each $N$ can be specified uniquely by
a set of $m$ additive quantities $(X_0, X_1, \cdots , X_{m-1})$, where
$$X_0 = U \quad (1)$$
is the internal energy. Let $(\hat{X}_{N,0}, \hat{X}_{N,1}, \cdots , \hat{X}_{N,m-1})$ be a set of the corresponding additive observables, where
$$\hat{X}_{N,0} = \hat{H}_N \quad (2)$$
is the Hamiltonian. Here, we do not include the interactions with external fields in the internal energy $U$ or the corresponding observable $\hat{H}_N$, as in the case of the MCE [62], because we choose additive quantities $(X_0, X_1, \cdots , X_{m-1})$, rather than the temperature and external fields, as independent thermodynamic parameters. Hereafter, we assume that all quantities are nondimensionalized using an appropriate scale.

To take the thermodynamic limit, we introduce an additive quantity per site
$$x_i \equiv X_i/N \quad (i = 0, 1, \cdots , m - 1). \quad (3)$$
It gives the average density in a phase coexisting state, while it is just the density in a homogeneous state, of the additive quantity. For simplicity, throughout this paper, we use the term “additive quantity density” even when two or more phases coexist. Particularly, $u \equiv U/N$ is the energy density. The corresponding observable is given by
$$\hat{x}_{N,i} \equiv \hat{X}_{N,i}/N \quad (i = 0, 1, \cdots , m - 1), \quad (4)$$
and we call it “additive observable density”. Particularly, we write $\hat{h}_N \equiv \hat{H}_N/N$.

For simplicity of notation, sets of $m$ physical quantities are denoted by bold symbols like
$$\mathbf{x} = (x_0, x_1, \cdots , x_{m-1}), \quad (5)$$
$$\hat{\mathbf{x}} = (\hat{x}_0, \hat{x}_1, \cdots , \hat{x}_{m-1}). \quad (6)$$
We also define the product of sets of physical quantities, $\mathbf{x}$ and $\mathbf{y}$, as
$$\mathbf{x} \cdot \mathbf{y} \equiv \sum_i x_i y_i. \quad (7)$$
The thermodynamic state space $\Omega$ is an open subset of $\mathbb{R}^m$, spanned by $\mathbf{x}$.

**B. Thermodynamic entropy density and genuine thermodynamic quantities**

Let $s_{TD}$ be the thermodynamic entropy density (in the thermodynamic limit). Since the thermodynamic entropy is defined purely thermodynamically, $s_{TD}$ exists uniquely regardless of microscopic details of the system such as the noncommutativity of $\mathbf{X}_N$.

According to thermodynamics, $s_{TD}$ is a function of $\mathbf{x}$, $s_{TD} = s_{TD}(\mathbf{x})$, which is concave in $\Omega$. Note that $s_{TD}$ is strictly concave except in first-order phase transition regions. On the other hand, in first-order phase transition regions $s_{TD}$ becomes linear in a certain direction(s) and therefore not strictly concave [13] [63]. This is the reason why the CE cannot give a phase coexistence state [29].

In addition, $s_{TD}$ is continuously differentiable everywhere in $\Omega$ [13] [63] [64]. We furthermore employ the standard assumption for systems with short-range interactions that $s_{TD}$ is also twice continuously differentiable [65].

We call $s_{TD}$ and its derivatives the ‘genuine thermodynamic quantities’. In particular, the first derivatives are the (entropic) intensive parameters [13]. We use $\Pi_i$ to denote the intensive parameter conjugate to $X_i$, i.e.,
$$\Pi_i(\mathbf{x}) \equiv \frac{\partial s_{TD}}{\partial x_i}(\mathbf{x}). \quad (8)$$
Particularly, $\beta(\mathbf{x}) \equiv \Pi_0(\mathbf{x})$ is the inverse temperature of the equilibrium state specified by $\mathbf{x}$.

**C. Canonical ensemble**

One way to obtain $s_{TD}$ from statistical mechanics is to use the canonical ensemble (CE), which is defined by
$$\hat{\nu}_N^c(\pi) \equiv \frac{e^{-N \pi \cdot \hat{x}_N}}{\text{Tr} \left[ e^{-N \pi \cdot \mathbf{x}_N} \right]}, \quad (9)$$
$$\psi^c_N(\pi) \equiv -\frac{1}{N} \log \text{Tr} \left[ e^{-N \pi \cdot \hat{\mathbf{x}}_N} \right], \quad (10)$$
where
$$\pi = (\pi_0, \pi_1, \cdots , \pi_{m-1}) \in \mathbb{R}^m \quad (11)$$
is the parameter of the CE and is equal to the set of intensive parameters $\Pi$ defined by Eq. (8). In the thermodynamics limit, the thermodynamic function
$$\psi^c(\pi) \equiv \lim_{N \to \infty} \psi^c_N(\pi) \quad (12)$$
given by the CE agrees with the Massieu function. Therefore, one can obtain the thermodynamic entropy density $s_{TD}$ by Legendre-Fenchel transforming $\psi^c$ [24]:
$$s_{TD}(\mathbf{x}) = \inf_{\pi} \left\{ \pi : \mathbf{x} - \psi^c(\pi) \right\}. \quad (13)$$
That is, although the CE fails to give the correct equilibrium state at the first-order transition region, it does give the correct thermodynamic function everywhere in the thermodynamic state space in the thermodynamics limit.

**III. DIFFICULTIES WITH NONCOMMUTATIVE ADDITIVE OBSERVABLES**

In this section, we briefly review the difficulties faced by conventional ensembles which have been employed to
analyze phase coexistence states, due to the noncommutativity of additive observables.

As discussed in Section I, to analyze phase coexistence states, the MCE and the RE, which are specified by the values of additive observables, have conventionally been employed. However, a straightforward generalization of such ensembles to the noncommutative case is ill-defined, or lead to pathological behavior of the density matrix in general.

To illustrate this point let us take a simple example of free spins, for which

\[ \hat{H}_N = \hat{X}_{N,0} = \sum_{i=1}^{N} \hat{\sigma}_{i}^x, \quad \text{(14)} \]

\[ \hat{X}_{N,1} = \sum_{i=1}^{N} \hat{\sigma}_{i}^y. \quad \text{(15)} \]

Obviously, \( \hat{X}_{N,0} \) and \( \hat{X}_{N,1} \) do not commute with each other. This gives rise to the following difficulties, and we cannot employ either the MCE or the RE, which are conventionally used in the analysis of classical systems with first-order phase transitions.

First, we consider the MCE. If \( \hat{x}_{N,0} \) and \( \hat{x}_{N,1} \) were able to be diagonalized simultaneously, the MCE could be defined as an equally weighted mixture of their simultaneous eigenstates \( \{x_0, x_1\} \) corresponding to eigenvalues \( (x_0, x_1) \) in a given two-dimensional interval \( I \subset \mathbb{R}^2 \), called the ‘shell’, and its density matrix could be given by

\[ \tilde{\rho}_N^\text{MC} \propto \sum_{(x_0, x_1) \in I} |x_0, x_1 \rangle \langle x_0, x_1|. \quad \text{(16)} \]

However, since \( \hat{x}_{N,0} \) and \( \hat{x}_{N,1} \) do not commute, the simultaneous eigenstates do not exist except when \( (x_0, x_1) = (0, 0) \) (which corresponds to the state with infinite temperature). Therefore, the density matrix of the MCE at finite temperature is ill-defined and impossible to construct.

Next, we consider the RE. Its density matrix has the following form [54]

\[ \tilde{\rho}_N^\text{RE} \propto \hat{P}_N e^{-\pi_0 \hat{X}_{N,0} \hat{P}_N}, \quad \text{(17)} \]

where \( \hat{P}_N \) is the projection operator onto the subspace spanned by the eigenstates of \( \hat{X}_{N,1} \) whose eigenvalues are in the range \( [m^-, m^+] \). Here we take \( m^\pm \) to be \( N \)-independent constants that satisfy \( 0 < m^- < m^- < 1 \). Then, \( \hat{x}_{N,0} \) has an anomalously large fluctuation in \( \tilde{\rho}_N^\text{RE} \). In fact, as proved in Appendix A the variance of \( \hat{x}_{N,0} \) in \( \tilde{\rho}_N^\text{RE} \) is \( \Theta(N^0) \) [67]:

\[ \lim_{N \to \infty} \text{Tr} \left[ \left( \hat{x}_{N,0} - x_{N,0}^r \right)^2 \tilde{\rho}_N^\text{RE} \right] \geq m^- (1 - m^-) \tanh^2 \pi_0, \quad \text{(18)} \]

where \( x_{N,0}^r = \text{Tr} [\hat{x}_{N,0} \tilde{\rho}_N^\text{RE}] \). However, it should be \( o(N^0) \) [63] if \( \tilde{\rho}_N^\text{RE} \) were a macroscopically definite state, such as a thermal equilibrium state. To make matters worse, \( \tilde{\rho}_N^\text{RE} \) contains superpositions of macroscopically distinct states with a significant magnitude [56]. That is, the state given by the RE is quite far from thermal equilibrium in general. As discussed in Ref. [56], the above argument holds similarly for interacting systems.

We solve these problems of the conventional ensembles by extending the SE to quantum systems whose equilibrium states are specified by a set of noncommutative additive observables. Although it might look straightforward extension of the SE that is specified only by the internal energy [29], its validity as a thermal ensemble is never obvious as we have seen for the MCE and RE and hence needs to be proved.

For this reason, we will clearly define the SE, derive useful formulas, and show their validity, for equilibrium states that are specified by a set of noncommutative additive observables.

### IV. SQUEEZED ENSEMBLE

Before describing detailed formulation, we explain the basic idea and the definitions of the SE in this section. We will prove various properties in the subsequent sections, whose main results are summarized in Sections VIII, VIII and VIII. We will also summarize the usage of the SE in Section VIII.

#### A. Basic Idea

When equilibrium states (for each \( N \)) are specified only by the internal energy \( U \), the density matrix of the SE is defined as [29]

\[ \tilde{\rho}_N^\text{SE}(\kappa) \propto e^{-N \eta(\kappa; h_N)}. \quad \text{(19)} \]

Here, \( \eta(\kappa; h) \) is the operator that is obtained by substituting the Hamiltonian density \( h \) for the internal energy \( u \) in a function \( \eta(\kappa; u) \), which is parametrized by an ensemble parameter \( \kappa \). Although the parameter \( \kappa \) is not a thermodynamic quantity, it specifies an equilibrium state uniquely [29]. By imposing several conditions on \( \eta(\kappa; u) \), such as the convexity, we proved in Ref. [29] that \( \tilde{\rho}_N^\text{SE}(\kappa) \) always gives the correct equilibrium state even in a first-order phase transition region.

To extend the SE to equilibrium states specified by noncommutative additive observables, we extend \( \eta(\kappa; u) \) to a function \( \eta(\kappa; x) \) of a set of the additive quantity densities \( x \), parametrized by a set of ensemble parameters \( \kappa \). The conditions on \( \eta(\kappa; u) \) are also extended to those on \( \eta(\kappa; x) \). The density matrix is obtained by substituting the additive observable densities \( \hat{x}_N \) for \( x \),

\[ \tilde{\rho}_N^\text{SE}(\kappa) \propto e^{-N \eta(\kappa; x_N)}. \quad \text{(20)} \]

In this substitution, the noncommutativity of \( \hat{x}_N \) should be treated appropriately. One way to define an operator function from a general real function is to use the
spectral decomposition. However, this method cannot be used in our case because \( \hat{x}_N \) cannot be diagonalized simultaneously. Hence, we take \( \eta(\kappa; \hat{x}) \) as a polynomial of \( \hat{x} \). (This can be generalized to a well-behaved power series of \( \hat{x} \).) In this case, \( \eta(\hat{x}_N) \) is given by the sum of products of \( \hat{x}_{N,i} \), and thus it does not require simultaneous eigenstates for its definition. Since \( \eta(\hat{x}_N) \) can be different depending on the order of the products of \( \hat{x}_{N,i} \) that appear when calculating \( \eta(\hat{x}_N) \), we let \( \eta(\kappa; \hat{x}) \) be a polynomial defined up to the order of the product. (Such a polynomial is generally called a ‘noncommutative polynomial’.) Although the order of the product needs to be specified to define the SE, it is irrelevant to the results obtained from the SE in the thermodynamic limit (see Section VI).

In addition, corresponding to the increase of the dimension of the thermodynamic state space \( \Omega \), we extend the ensemble parameter from a single real number \( \kappa \) to a set of real numbers

\[
\kappa = (\kappa_0, \kappa_1, \cdots, \kappa_{p-1}). \tag{21}
\]

It is natural to take the number \( p \) of the parameters to be the same as the dimension \( m \) of the thermodynamic state space \( \Omega \), but it is not necessarily the same and can be greater than \( m \):

\[
m \leq p \tag{22}
\]

We write \( K (\subset \mathbb{R}^p) \) for the space formed by the parameter \( \kappa \).

### B. Definition of the SE

Based on the above idea, we introduce the SE as a general class of ensembles which give equilibrium values of local observables, additive observables, and the genuine thermodynamic quantities even when equilibrium states are specified by noncommutative additive observables.

Let \( \eta(\kappa; \hat{x}) \) be a noncommutative polynomial (or well-behaved power series \( \left[ 69 \right] \)) with real coefficients in \( m \) noncommutative variables \( \hat{x} \), parametrized by \( p \) real numbers \( \kappa \) in \( K \). We define the squeezed ensemble (SE) associated with \( \eta \) by

\[
\hat{\rho}_N^\eta(\kappa) \equiv \frac{e^{-N\eta(\kappa; \hat{x}_N)}}{\text{Tr} \left( e^{-N\eta(\kappa; \hat{x}_N)} \right)} \tag{23}
\]

and write the normalization constant as

\[
\psi_N^\eta(\kappa) \equiv -\frac{1}{N} \log \text{Tr} \left( e^{-N\eta(\kappa; \hat{x}_N)} \right) \tag{24}
\]

Note that simultaneous eigenstates of \( \hat{X}_N \) do not appear in the definition of the SE. Therefore, the SE is well-defined even in the case where \( \hat{X}_N \) cannot be diagonalized simultaneously.

Since \( \eta \) is defined for noncommutative variables, it is possible to substitute the commutative quantities for the variables as a special case. Therefore, the polynomial \( \eta \) defines a real function on \( \mathbb{R}^m \) uniquely. When there is no danger of confusion, we will use the same symbol \( \eta \) for this function. Using this notation, we impose the following four conditions on \( \eta \).

(A) \( \eta(\kappa; \hat{x}_N) \) is self-adjoint for all \( \kappa \in K \) and \( N \).

(B) \( s_{\operatorname{TD}}(x) - \eta(\kappa; x) \) has the unique maximum point \( x_{\text{max}}^\eta \) in \( \Omega \) and is strongly concave in a neighborhood of \( x_{\text{max}}^\eta \) for all \( \kappa \in K \).

(C) \( \eta(\kappa; x) \) is twice continuously differentiable as a \( (p+m) \)-variable function of \( \kappa \) and \( x \).

(D) \( x_{\text{max}}^\eta(\kappa) \) is surjective onto \( \Omega \).

Before going into details, we briefly explain physical meanings of these conditions. The condition \( \left[ A \right] \) ensures that \( \hat{\rho}_N^\eta(\kappa) \) is a density matrix. Since all additive observable densities \( \hat{x}_{N,i} \) are self-adjoint, this condition can be easily satisfied by employing an appropriately symmetrized polynomial as \( \eta \). The condition \( \left[ B \right] \) ensures that all additive observables that specify the equilibrium state have macroscopically definite value in the SE. By contrast, as discussed in Section I at the first-order phase transition point, the CE gives a statistical mixture of macroscopically distinct states in many cases. This condition makes the SEs free from such deficiency. Since \( s_{\operatorname{TD}} \) is concave, this condition is always satisfied when \( \eta \) is taken as a strongly convex function. The condition \( \left[ C \right] \) ensures that the equilibrium state described by the SE changes continuously with respect to the parameter \( \kappa \). The condition \( \left[ D \right] \) plays a crucial role for obtaining all thermodynamic properties from the thermodynamic function given by the SE.

### V. BASIC PROPERTIES WHEN \( \hat{X}_N \) IS COMMUTATIVE

In this and the next section, we investigate the basic properties of the SE when the parameter \( \kappa \) is fixed to an arbitrary set of values, and hence we simplify notation by abbreviating \( \eta(\kappa; \hat{x}) \) as \( \eta(\hat{x}) \) except for the final results (which are displayed in frames).

We first discuss the simple case where \( \hat{X}_N \) commute with each other in this section. The noncommutative case will be discussed in the next section.

#### A. Basic properties of density matrix of the SE

We examine the probability distribution \( \hat{\rho}_N^\eta(x) \) of the additive quantity densities \( x \) in \( \hat{\rho}_N^\eta \).

Since we are considering the commutative case in this section, \( \hat{X}_N \) can be diagonalized simultaneously, and we can thereby define the density of microstates. We divide the thermodynamic state space \( \Omega \) (more precisely, \( \mathbb{R}^m \))
into a direct sum of $m$-dimensional intervals $I_n$ of side lengths of $o(N^0)$ and write $g_N(x)$ for the density of macrostates averaged within the interval $I_n$ that contains $x \in \Omega$. By Boltzmann’s entropy formula, the logarithm of $g_N$ approaches the thermodynamic entropy $s_{TD}$ in the thermodynamic limit (TDL):

$$\sigma_N(x) \equiv \frac{1}{N} \log g_N(x) \xrightarrow{TDL} s_{TD}(x). \quad (25)$$

From this relation, for any smooth function $f(x)$ we have

$$\text{Tr} \left[ f(\hat{x}_N) e^{-N\eta(\hat{x}_N)} \right] = \int dx g_N(x) f(x) e^{-N[\eta(x)+o(N^0)]}$$

$$= \int dx f(x) e^{N[s_{TD}(x) - \eta(x)+o(N^0)]}$$

= \int dx f(x) e^{N[s_{TD}(x)-\eta(x)+o(N^0)]}.

Therefore, we obtain

$$p_N^x(x) \propto e^{N[s_{TD}(x)-\eta(x)+o(N^0)]}. \quad (26)$$

From condition (B) the function $s_{TD}(x) - \eta(x)$ in the exponential has the unique maximum at $x_{\text{max}}^N$, which satisfies

$$\frac{\partial s_{TD}}{\partial x_i}(x_{\text{max}}^N) = \frac{\partial \eta}{\partial x_i}(x_{\text{max}}^N). \quad (28)$$

We investigate properties of $p_N^x(x)$ in the vicinity of this maximum point. Expanding $s_{TD}(x) - \eta(x)$ around $x_{\text{max}}^N$, we get

$$s_{TD}(x) - \eta(x)$$

= $s_{TD}(x_{\text{max}}^N) - \eta(x_{\text{max}}^N)$

$$- \frac{1}{2} \sum_{i,j} (x_i - x_{\text{max}}^N,i)(-H_{ij})(x_j - x_{\text{max}}^N,j) + \cdots, \quad (29)$$

where $H$ is the Hesse matrix of $s_{TD}(x) - \eta(x)$ at $x_{\text{max}}^N$:

$$H_{ij} = \frac{\partial^2 s_{TD}}{\partial x_i \partial x_j}(x_{\text{max}}^N) - \frac{\partial^2 \eta}{\partial x_i \partial x_j}(x_{\text{max}}^N). \quad (30)$$

Again from condition (B), the matrix $H$ is negative definite. Hence, $e^{N[s_{TD}(x)-\eta(x)]}$ behaves as the Gaussian distribution in the vicinity of $x_{\text{max}}^N$, peaking at $x_{\text{max}}^N$, with the covariance matrix $-N^{-1}H^{-1}$:

$$\exp \left[ -\frac{1}{2} \sum_{i,j} (x_i - x_{\text{max}}^N,i)(-NH_{ij})(x_j - x_{\text{max}}^N,j) \right]. \quad (31)$$

Although higher-order terms are dropped in this equation (Laplace’s approximation [21]), their contributions become negligible in the thermodynamic limit because we have taken $s_{TD}(x) - \eta(x)$ strongly concave. Taking also the $o(N^0)$ term in $p_N^x(x)$ into account, we obtain

$$\text{Tr} [f(\hat{x}_N) p_N^x(x)] = f(x_{\text{max}}^N) + o(N^0). \quad (32)$$

Letting $f(x) = x_i$ in Eq. (32), we obtain the expectation value of $\hat{x}_N$ as

$$x_{\text{max}}^N(\kappa) \equiv \text{Tr} [\hat{x}_N \hat{\rho}_N^x(\kappa)] \rightarrow x_{\text{max}}^N(\kappa) \quad (33)$$

Furthermore, letting $f(x) = (x_i)^2$ in Eq. (32) and combining it with Eq. (33), we obtain the variance as

$$\lim_{N \rightarrow \infty} \text{Tr} \left[ (\hat{x}_N - x_{\text{max}}^N(\kappa))^2 \hat{\rho}_N^x(\kappa) \right] = 0 \quad (34)$$

That is, in the density matrix given by the SE, all $\hat{x}_N,i$ have macroscopically definite values. This is in contrast to the CE, in which some $\hat{x}_N,i$ has macroscopically large fluctuation at the first-order phase transition point.

Moreover, $\hat{\rho}_N^x$ can be characterized by the principle of equal probability. That is, under the constraint of

$$\text{Tr} [\eta(\hat{x}_N) \hat{\rho}] = \text{Tr} [\eta(\hat{x}_N) \hat{\rho}_N^x], \quad (35)$$

we can show that the density matrix $\hat{\rho}$ that maximizes the von Neumann entropy,

$$S_{\text{vN}}(\hat{\rho}) = -\text{Tr} [\hat{\rho} \log \hat{\rho}], \quad (36)$$

exists uniquely and is equal to $\hat{\rho}_N^x$, from argument similar to that of Refs. [72][74]. Note that this argument can also be applied to the case where $\hat{X}_N$ do not commute with each other.

From these results, we conclude that the density matrix $\hat{\rho}_N^x$ given by the SE gives typical properties of the macrostates in which additive quantity densities $x$ are $x_{\text{max}}^N$. Therefore, by choosing $\eta$ such that $x_{\text{max}}^N$ coincides with $x$ in the particular equilibrium state of interest, one can obtain the quantum state corresponding to that equilibrium state. In particular, by choosing $\eta$ such that $x_{\text{max}}^N$ lies within the first-order phase transition region, one can obtain a phase coexistence state without finding and imposing clever boundary conditions according to the phases to be coexisted as in the case of using the CE. Thus, by using the SE, one can investigate microscopic structures of phase coexisting states, such as the phase interfaces.

**B. Genuine thermodynamic quantities**

We can also obtain genuine thermodynamic quantities, such as the thermodynamic entropy density and the intensive parameter, easily from the SE.

First, we derive a formula for the thermodynamic entropy density. We note that only $x$ which is in close vicinity around the peak position $x_{\text{max}}^N$ contributes to the integral in the right hand side of Eq. (26). Hence,
Therefore, we obtain

\[ \text{Tr} \left[ e^{-N\eta(\hat{x}_N)} \right] = \frac{(2\pi)^{m/2}}{N^{m/2}|H|^{1/2}} e^{N[s_{TD}(\mathbf{x}_{\text{max}}^\eta)-\eta(\mathbf{x}_{\text{max}}^\eta)+o(N^0)]} \{ 1 + o(N^0) \} . \]

(37)

Here \( |H| \) is the determinant of the Hesse matrix \( H \). Then we obtain

\[ \psi_N^\eta = -\frac{1}{N} \log \text{Tr} \left[ e^{-N\eta(\hat{x}_N)} \right] = \eta(\mathbf{x}_{\text{max}}^\eta) - s_{TD}(\mathbf{x}_{\text{max}}^\eta) + o(N^0). \]

(38)

Therefore, we obtain

**Property (when \( \hat{X}_N \) is commutative) 3.**

\[ s_N^\eta(\kappa) \equiv \eta(\kappa; \mathbf{x}_N^\eta(\kappa)) - \psi_N^\eta(\kappa) \rightarrow s_{TD}(\mathbf{x}_{\text{max}}^\eta(\kappa)) \]  

(39)

Since \( \eta \) is a known function, one can obtain the thermodynamic entropy density from \( \mathbf{x}_N^\eta \) and \( \psi_N^\eta \) using this formula.

Next, we derive a formula for intensive parameters. Using Eq. (28) and in the same manner as above, we also obtain

**Property (when \( \hat{X}_N \) is commutative) 4.**

\[ \Pi_{N,i}^\eta(\kappa) \equiv \frac{\partial \eta}{\partial x_i}(\kappa; \mathbf{x}_N^\eta) \rightarrow \Pi_i(\mathbf{x}_{\text{max}}^\eta(\kappa)) \]  

(40)

Since \( \eta \) is a known function, using this formula, one can obtain the intensive parameters just by calculating \( \mathbf{x}_N^\eta \). This is a great advantage of the SE over the MCE. Since we consider the commutative case in this section, the MCE is well defined (unlike the noncommutative case). However, one needs to differentiate the entropy in order to calculate the intensive parameters from the MCE, and it gives very noisy results in numerical calculation. One can avoid such noisy calculation by using formula Eq. (40) of the SE.

### C. Summary of properties when \( \hat{X}_N \) is commutative

We have discussed the case where \( \hat{X}_N \) is commutative in this section. By using the SE, one can correctly obtain the desired phase coexistence states without any ad hoc procedures, such as devising boundary conditions. One can also obtain genuine thermodynamic quantities, such as the thermodynamic entropy density and the intensive parameter, easily from the SE. Therefore, one can investigate microscopic structures and thermodynamic properties of phase coexistence states.

In the next section, we will show that all these properties are kept even in the noncommutative case.

### VI. BASIC PROPERTIES WHEN \( \hat{X}_N \) IS NONCOMMUTATIVE

We now study the noncommutative case. As in the previous section, we fix \( \kappa \) to an arbitrary set of values and abbreviate \( \eta(\kappa; \mathbf{x}) \) as \( \eta(\mathbf{x}) \) except for the final results.

#### A. Strategy for proofs and derivations

When \( \hat{X}_N \) do not commute with each other, the density of microstates \( g_N(\mathbf{x}) \) is ill-defined. Hence, we cannot apply the arguments, such as Laplace’s approximation, of the previous section directly.

To overcome this obstacle, we bring the idea proposed by von Neumann of using a commutative set of observables \( \hat{x}_N \) that approximate the set of additive observable densities \( \hat{x}_N \). Although such a set of commutative observables are hard to construct, we use it only for the proofs and derivations of the basic properties of the SE, assuming only the existence of \( X_N \).

After establishing the validity and formulas of the SE, we can use the set of original additive observable densities \( \hat{x}_N \) when applying the SE to concrete calculations. That is, we can calculate statistical-mechanical quantities without using \( \hat{x}_N \), which would be practically impossible to construct.

#### B. Commutative set of observables that approximates \( X_N \)

Let us introduce the commutative set of observables \( \hat{x}_N \). Since we are considering a general quantum spin system, its local Hilbert space on each site is taken as \( \mathbb{C}^d \). The spins are located on the \( \nu \)-dimensional hypercubic lattice, denoted by \( \Lambda_n = [-n,+n]^\nu \cap \mathbb{Z}^\nu \). Then, an additive observable \( \hat{X}_{N,i} \) is expressed as

\[ \hat{X}_{N,i} = \sum_{j \in \mathbb{Z}^\nu} \gamma_j(\delta_i), \]

(41)

where \( \gamma_j \) is the \( j \)-lattice translation for \( j \in \mathbb{Z} \) and \( \delta_i \) is an \( N \)-independent local observable with support \( I_i \). For this system, Ogata [60] proved that there exists a set of \( m \) observables

\[ \hat{x}_N = (\hat{x}_{N,0}, \hat{x}_{N,1}, \cdots, \hat{x}_{N,m-1}) \]

(42)

such that

\[ \lim_{N \to \infty} \| \hat{x}_{N,i} - \hat{x}_{N,i} \| = 0 \quad (i = 0, 1, \cdots, m-1), \]

(43)

\[ [\hat{x}_{N,i}, \hat{x}_{N,j}] = 0 \quad (i, j = 0, 1, \cdots, m-1). \]

(44)
To put it differently, there exists a commutative set of observables \( \xi_N \) that approximates a noncommutative set of additive observable densities \( \hat{x}_N \) in the thermodynamic limit.

For notational simplicity, we use the notation \( \bullet \) to represent the quantity \( \bullet \) associated with \( \hat{x}_N \) and the quantity \( \dot{\bullet} \) associated with \( \dot{x}_N \) together. Using this notation, we define two types of SEs, one for \( \hat{x}_N \) and the other for \( \dot{x}_N \), as

\[
\rho_{\eta}^\hat{x} = \frac{e^{-N\eta(\hat{x}_N)}}{\text{Tr}[e^{-N\eta(\hat{x}_N)}]},
\]

\[
\psi_{\eta}^\hat{x} = -\frac{1}{N} \log \text{Tr}[e^{-N\eta(\hat{x}_N)}],
\]

where \( \hat{x}_N = \hat{x}_N \) or \( \hat{x}_N \). For the expectation value, we write

\[
\langle \bullet \rangle_{\eta}^\hat{x} = \text{Tr}\left[\bullet \rho_{\eta}^\hat{x}\right].
\]

We prove the following two theorems in Appendices B and C.

First, the thermodynamic function given by the SE for \( \hat{x}_N \) coincides with that given by the SE for \( \dot{x}_N \):

**Theorem 1.** If \( \psi_{\eta}^\hat{x} \) and \( \psi_{\eta}^{\dot{x}} \) converge in the thermodynamic limit, then

\[
\lim_{N \to \infty} \psi_{\eta}^\hat{x} = \lim_{N \to \infty} \psi_{\eta}^{\dot{x}}.
\]

This holds even when condition \([B]\) is not satisfied.

In the proof we use only the fact that \( \eta \) satisfies condition \([A]\) and is Lipschitz continuous in the operator norm. Since condition \([B]\) is unnecessary, this theorem holds even for \( \eta = \pi \cdot \hat{x} \), which associates the CE (see Section VII A) and does not satisfy condition \([B]\) at the phase transition point. This fact will be crucial when deriving formulas for the genuine thermodynamic quantities in Section V T C.

Next, we consider the expectation values of observables. Here, we focus on observables, especially those that can be expressed as polynomials (denoted as \( \theta \)) of the observables \( \hat{x} \). This class of observables includes not only \( \hat{x}_{N,i} \), but also their higher-order moments. We obtain the following theorem:

**Theorem 2.** Let \( \theta \) be a polynomial with real coefficients in \( m \) noncommutative variables. We assume that \( \theta \) is independent of \( N \) and that \( \theta(\hat{x}_N) \) is self-adjoint for all \( N \).

If the following conditions are fulfilled:

(i) \( \{\langle \theta(\hat{x}_N)\rangle_{\eta}^\hat{x}\}_{N \in \mathbb{N}} \) and \( \{\langle \theta(\hat{x}_N)\rangle_{\eta}^{\dot{x}}\}_{N \in \mathbb{N}} \) converge in the thermodynamic limit,

(ii) There exists a closed and bounded interval \( I \)

containing 0 and \( M > 0 \) such that, for any \( \lambda \in I \) and \( N \in \mathbb{N} \), the variance of \( \theta(\hat{x}_N) \) in the SE associated with \( \eta + \lambda \theta \) for \( \dot{x}_N \) satisfies

\[
\text{Tr}\left[\left(\theta(\hat{x}_N) - \langle \theta(\hat{x}_N)\rangle_{\eta}^{\dot{x}}(\lambda)\right)^2 \rho_{\eta}^{\dot{x}}(\lambda)\right] < \frac{M}{N},
\]

where

\[
\rho_{\eta}^{\dot{x}}(\lambda) = \frac{e^{-N(\eta(\hat{x}_N) + \lambda \theta(\hat{x}_N))}}{\text{Tr}[e^{-N(\eta(\hat{x}_N) + \lambda \theta(\hat{x}_N))}]},
\]

\[
\psi_{\eta}^{\dot{x}}(\lambda) \equiv \text{Tr}\left[\bullet \rho_{\eta}^{\dot{x}}(\lambda)\right],
\]

then we have

\[
\lim_{N \to \infty} \langle \theta(\hat{x}_N)\rangle_{\eta}^{\dot{x}} = \lim_{N \to \infty} \langle \theta(\hat{x}_N)\rangle_{\eta}^{\dot{x}}.
\]

These two theorems show that the statistical-mechanical properties of the SE are identical for \( \hat{x}_N \) and for \( \dot{x}_N \) in the thermodynamic limit.

Since condition \([B]\) is on the SE for the commutative observables \( \hat{x}_N \), it can be shown to hold using Laplace’s approximation under condition \([B]\) and assumptions listed in Section V T C as we do in Appendix D.

### C. Assumptions

Since \( \hat{x}_N \) can be diagonalized simultaneously, we can define the density of microstates that have the specified value of \( \hat{x}_N \). We write \( \tilde{g}_N \) for the density of microstates averaged in the same way as we defined \( g_N \) in Section V A. It is expected that \( \tilde{g}_N(\hat{x}) \) has the same properties as the density of microstates of the commutative case, \( g_N(\hat{x}) \). We therefore make the following reasonable assumptions:

1. There exists a concave function \( \varsigma(\hat{x}) \) such that

\[
\varsigma_N(\hat{x}) \equiv \frac{1}{N} \log \tilde{g}_N(\hat{x}) \xrightarrow{\text{TDL}} \varsigma(\hat{x}).
\]

2. Laplace’s approximation, which will be applied in Section V D in the same way as done in Section V for the SE constructed from \( \hat{x}_N \) gives exact results in the thermodynamic limit.

Let us discuss the validity of these assumptions. As pointed out by von Neumann in Ref. [57], in macroscopic experiments, it is possible to measure a set of macroscopic quantities simultaneously, and the observables measured are not \( \hat{x}_N \) but a set of “coarse-grained” commutative observables. The microcanonical entropy density for such a set of actually measured macroscopic observables should be \( \varsigma_N \). Therefore, it is expected that
\( \varsigma_N \) asymptotically approaches the thermodynamic entropy density \( s_{\text{TD}} \), which is concave, in the thermodynamic limit. In fact, we will show in Section VI C that \( \varsigma = s_{\text{TD}} \) under assumptions 1 and 2. Thus assumption 1 is reasonable.

Assumption 2 also seems to hold unless \( \varsigma_N \) exhibits very pathological behavior. Under assumption 1, \( \varsigma_N(x) - \eta(x) \) converges to \( \varsigma(x) - \eta(x) \), which is strongly concave because of condition (15). Hence, it is expected that \( \varsigma_N(x) - \eta(x) \) is also strongly concave, at least in the very vicinity of the peak position unless \( \varsigma_N \) exhibits pathological behavior in the region (such as having a point at which convergence to the thermodynamic limit is extremely slow). This corresponds to the fact that \( \sigma_N(x) - \eta(x) \) can be well approximated by the strongly concave function \( s_{\text{TD}}(x) - \eta(x) \) in the commutative case, discussed in Section VA in which Laplace’s approximation gives exact results in the thermodynamic limit. Therefore, we expect that Laplace’s approximation also works well in the case of \( \varsigma_N(x) - \eta(x) \).

D. Properties of the SE for commutative set \( X_N \)

Following the strategy explained in Section V A, we first study the basic properties of the SE for a commutative set \( \hat{x}_N \).

In preparation, we first discuss the relation between \( \varsigma \) and \( s_{\text{TD}} \). Using \( \varsigma_N \), the thermodynamic function given by the CE for \( \hat{x}_N \) can be expressed as

\[
\psi_N^\varsigma(\pi) = -\frac{1}{N} \log \text{Tr} \left[ e^{-N \pi \cdot \hat{x}_N} \right] = -\frac{1}{N} \log \int d\hat{x} e^{-N [\pi \cdot \hat{x} - \varsigma_N(\hat{x})]} + o(N^0). \tag{54}
\]

Since \( e^{-N [\pi \cdot \hat{x} - \varsigma_N(\hat{x})]} \) has its maximum value at the point where \( \pi \cdot \hat{x} - \varsigma_N(\hat{x}) \) is minimum and decreases exponentially away from the point, we find

\[
\psi_N^\varsigma(\pi) = \inf_{\hat{x} \in \Omega} \{ \pi \cdot \hat{x} - \varsigma_N(\hat{x}) \} + o(N^0). \tag{55}
\]

Therefore, in the thermodynamic limit, by using Theorem 1 for \( \eta = \pi \cdot \hat{x} \), we obtain

\[
\psi^\varsigma(\pi) = \lim_{N \to \infty} \psi_N^\varsigma(\pi) = \lim_{N \to \infty} \psi_N^\varsigma(\pi) = \inf_{\hat{x} \in \Omega} \{ \pi \cdot \hat{x} - \varsigma(\hat{x}) \}. \tag{56}
\]

Therefore, by Legendre-Fenchel transforming [23] both sides and using Eq. (15), we get

\[
\varsigma(\hat{x}) = s_{\text{TD}}(\hat{x}). \tag{57}
\]

Now we examine the probability distribution \( p_N^\eta(x) \) of the commutative set \( \hat{x}_N \) in the density matrix \( \rho_N^\eta \). Using Eq. (57), for any smooth function \( f(x) \), we have

\[
\text{Tr} \left[ f(\hat{x}_N)e^{-N(\eta(\hat{x}_N))} \right] = \int dx f(x)e^{N[\varsigma_N(x) - \eta(x) + o(N^0)]} = \int dx f(x)e^{N[s_{\text{TD}}(x) - \eta(x) + o(N^0)]}. \tag{58}
\]

This is just Eq. (20). Therefore, the results for \( p_N^\eta \) derived in Section V (Eqs. (27)-(31)) hold for \( p_N^\eta \) in the SE for \( \hat{x}_N \) as well. Then, evaluating the statistical-mechanical quantities in the SE for \( \hat{x}_N \), we obtain

\[
\lim_{N \to \infty} (f(\hat{x}_N))^\eta_N = f(x_{\text{max}}^\eta), \tag{59}
\]

\[
\lim_{N \to \infty} \psi_N^\eta = \eta(x_{\text{max}}^\eta) - s_{\text{TD}}(x_{\text{max}}^\eta), \tag{60}
\]

where \( x_{\text{max}}^\eta \) is the unique maximum point of \( s_{\text{TD}}(x) - \eta(\kappa; x) \).

E. Properties of the SE for noncommutative set \( X_N \)

Using the theorems presented in Section VI B, we derive properties of the SE for the noncommutative set \( \hat{x}_N \) from those of the SE for the commutative set \( \hat{x}_N \) in Appendix D. Here, we present the results and their implications.

First, we find that, as in the commutative case, the expectation value of \( \hat{x}_N \) approaches \( x_{\text{max}}^\eta \):

\[
x_{\text{N},i}^\eta(\kappa) \equiv \text{Tr} \left[ \hat{x}_{N,i}^\eta \rho_N^\eta(\kappa) \right] \xrightarrow{\text{TDL}} x_{\text{max},i}^\eta(\kappa) \tag{61}
\]

Furthermore, we obtain the variance as

\[
\lim_{N \to \infty} \text{Tr} \left[ (\hat{x}_{N,i} - x_{\text{max},i}^\eta)^2 \rho_N^\eta(\kappa) \right] = 0 \tag{62}
\]

That is, all \( \hat{x}_{N,i} \) have macroscopically definite values in the SE even when they are noncommutative. This is in contrast to the CE, in which some \( \hat{x}_{N,i} \) has macroscopically large fluctuation at the first-order phase transition point.

We can also show that the density matrix of the SE can be characterized by the principle of equal probability that was explained in Section V because the argument is also valid for the noncommutative case.

From these results, it is concluded that the density matrix \( \rho_N^\eta \) given by the SE gives typical properties of the microstates with \( x = x_{\text{max}}^\eta(\kappa) + o(N^0) \). Therefore, it gives the equilibrium state specified by \( x_{\text{max}}^\eta(\kappa) \). Moreover, we
will show in the next section that $x_{\text{max}}^\eta(\kappa)$ changes continuously as a function of $\kappa$. Hence, by choosing $\kappa$ such that $x_{\text{max}}^\eta(\kappa)$ lies within a first-order phase transition region, one can obtain a phase coexistence state. Thus, by using the SE, one can investigate microscopic structures of phase coexisting states, such as the phase interfaces.

Furthermore, the thermodynamic entropy density is obtained by the following formula:

\begin{equation}
\Pi^\eta(\kappa) \equiv \frac{\partial \eta(\kappa; x^\eta_N(\kappa))}{\partial x_i} \text{TDL} \Pi(x_{\text{max}}^\eta(\kappa)).
\end{equation}

Since $\eta$ is a known function, one can obtain the intensive parameters just by calculating the expectation value $x^\eta_N$, without differentiating thermodynamic functions.

F. Summary of properties when $X_N$ is noncommutative

To summarize this section, all the properties derived in Section $\$\$ for the case where a set of additive observables $X_N$ is commutative hold similarly for the case where $X_N$ is noncommutative. In addition, the density matrix of the SE can be characterized by the principle of equal probability. Therefore, by using the SE, we can correctly obtain the desired phase coexistence states of general quantum systems without any ad hoc procedures, such as devising boundary conditions. We can also obtain genuine thermodynamic quantities, such as the thermodynamic entropy density and the intensive parameter, easily from the SE. Therefore, one can investigate microscopic structures and thermodynamic properties of phase coexistence states of general quantum systems.

VII. PARAMETER OF SQUEEZED ENSEMBLE

So far, we have investigated the properties when the parameter $\kappa$ is fixed to an arbitrary set of values. We now discuss the $\kappa$ dependencies of the statistical-mechanical quantities given by the SE, under conditions $\$\$ and $\$\$. We will show that the equilibrium state described by the SE changes continuously with respect to the parameter $\kappa$ (Section $\$\$) and that the thermodynamic function obtained from the SE is related to the thermodynamic entropy $s_{\text{TDL}}$ via a generalization of the Legendre-Fenchel transformation (Section $\$\$). We will also discuss connection with conventional generalized ensembles (Section $\$\$).

A. CE

Suppose that the system does not undergo a phase transition, so that its thermodynamic entropy density $s_{\text{TDL}}$ is strongly concave. In this case, we can take $\eta$ as a linear function, $\eta(\kappa; x) = \kappa \cdot x$, which reduces to the CE. Therefore, the CE can be regarded as a special form of the SE when a phase transition is absent.

To distinguish the CE from the general SEs, we write $c$ and $\pi = (\pi_0, \ldots, \pi_{m-1})$ for $\eta$ and $\kappa$ of the CE, respectively. That is, $\eta$ for the CE is denoted as

\begin{equation}
c(\pi; x) = \pi \cdot x.
\end{equation}

Then it is seen from Eq. (64) that

\begin{equation}
\pi_i = \Pi_i(x_{\text{max}}^c(\pi)).
\end{equation}

This equation simply states that the intensive parameters $\Pi$ in the equilibrium state specified by $\pi$ are just $\pi$, as they should be.

In this particular case, $\kappa$ coincides with the thermodynamic quantities $\Pi$. For general SEs, however, $\kappa$ is not directly related to the thermodynamic quantities. Nevertheless, one can calculate thermodynamic quantities from the SEs via Eqs. (70) and (71) as shown below, as well as via Eqs. (63) and (64).

B. Parameter dependence of the density matrix of the SE

We consider the parameter dependence of the equilibrium state described by the SE. As shown in Sections $\$\$ and $\$\$ the equilibrium state described by the SE is specified by $x_{\text{max}}^\eta$ in the thermodynamic limit. Hence, we investigate the $\kappa$ dependence of $x_{\text{max}}^\eta$, i.e., the function $x_{\text{max}}^\eta(\kappa)$.

Since $x_{\text{max}}^\eta$ is the maximum point of the strongly-concave function $s_{\text{TDL}}(x) - \eta(\kappa; x)$, it is uniquely determined by

\begin{equation}
F_i(\kappa; x_{\text{max}}^\eta) = 0 \quad (i = 0, 1, \ldots, m - 1),
\end{equation}

where

\begin{equation}
F_i(\kappa; x) = \frac{\partial s_{\text{TDL}}}{\partial x_i}(x) - \frac{\partial \eta}{\partial x_i}(\kappa; x) \quad (i = 0, 1, \ldots, m - 1).
\end{equation}

From condition $\$\$ $F_i$ is a continuously differentiable function of $\kappa$ and $x$. Hence, applying an implicit function theorem $\$\$, we find
Therefore, the equilibrium state described by the SE changes continuously as a function of $\kappa$.

This should be contrasted with the CE at a first-order phase transition point. In that case, since condition [15] is not satisfied, the CE is not an SE and $x^{c}_{\text{max}}$ is not unique. Consequently, as passing through the first-order phase transition point, $x^{c}_{\text{max}}$ switches discontinuously. This means that the equilibrium state described by the CE changes discontinuously as a function of $\pi$. Therefore, the CE is unable to describe the equilibrium states in the first-order phase transition region. Property 5 implies that such a discontinuous change does not occur in the SE.

**Property 6.** For all $x \in \Omega$, we have

$$s_{TD}(x) = \inf_{\kappa \in K} \{ \eta(\kappa; x) - \psi^{\eta}(\kappa) \} \quad (71)$$

Using this relation, one can obtain the thermodynamic entropy $s_{TD}(x)$ directly from $\psi^{\eta}(\kappa)$ without knowing the function $x^{\eta}(\kappa)$. In this sense, $\psi^{\eta}(\kappa)$ is equivalent to the thermodynamic entropy. Therefore, all thermodynamic functions are obtained from $\psi^{\eta}(\kappa)$.

From a physical point of view, relation [70]-[71] is a generalization of the equivalence of the entropy and the canonical thermodynamic function. From a mathematical point of view, the relation is a generalization of the Legendre-Fenchel transformation.

**D. Connection with the conventional generalized ensembles**

Here we mention the connection with the conventional generalized ensembles.

Consider the SE for the particular choice of $\eta$,

$$\eta(\kappa; x) = \kappa \cdot x + g(x), \quad (72)$$

where $g$ is a continuous function that is fixed independently of $\kappa$. This $\eta$ defines the so-called generalized canonical ensemble introduced by M. Costeniuc et al. [23, 24]. It includes generalized ensembles introduced in earlier studies such as the Gaussian ensemble, which is obtained by taking $g$ as

$$g(x) = \gamma \sum_{i} x_{i}^{2}, \quad (73)$$

where $\gamma$ is a fixed positive constant independent of $\kappa$. In fact, this choice of $g$ gives the density matrix that can be written as

$$\hat{\rho}_{N}^{\eta}(\kappa) \propto \exp \left[ -N \gamma \sum_{i} \left( \hat{x}_{N,i} + \frac{\kappa_{i}}{2\gamma} \right)^{2} \right], \quad (74)$$

which has the same form as the Gaussian ensemble originally proposed by Hetherington [14, 15, 17, 23].

In the generalized canonical ensemble, Eq. (72), the parameter $\kappa_{i}$ couples with $x_{i}$ linearly in order for $s_{TD}(u) - g(u)$ to be the Legendre-Fenchel transform of the thermodynamic function given by the ensemble. Therefore, in quantum systems, it is necessary to compute the matrix exponential each time the parameters are changed. In numerical calculations, the matrix exponential is usually evaluated by utilizing the Suzuki-Trotter decomposition, but this method has drawbacks such as the Trotter error.

In comparison, the parameter dependence is more general in the SE. Even when $\kappa_{i}$ couples with $x_{i}$ nonlinearly the thermodynamic function given by the SE is equivalent to the thermodynamic entropy as shown in Section VII C. This generality allows us to choose $\eta$ that is greatly convenient for practical use.

To illustrate this point let us take a simple example of the case where the equilibrium state is specified only by the internal energy (i.e., $m = 1$). We can take $\eta = -2k_{0} \log(l - x_{0})$ and $K = (0, \infty)$, where $l$ is an arbitrary constant such that $NI \geq$ the largest eigenvalue of $\tilde{H}_{N}$ [29, 77]. This choice of $\eta$ is particularly convenient for quantum systems, because a series of density matrices given by the SE

$$\hat{\rho}_{N}^{\eta}(\kappa_{0} = k/N) \propto (NI - \tilde{H}_{N})^{2k} \quad (k = 0, 1, 2, \cdots) \quad (75)$$

can be constructed sequentially by simply multiplying $(NI - \tilde{H}_{N})$ repeatedly:

$$\hat{\rho}_{N}^{\eta}((k + 1)/N) \propto (NI - \tilde{H}_{N})^{2} \times \hat{\rho}_{N}^{\eta}(k/N). \quad (76)$$

Therefore, when using this SE, the calculation of the matrix exponential, which is unavoidable when using the generalized canonical ensemble, is no longer necessary. Although the SEs that can be constructed in this way are limited to those at discrete points $\kappa_{0} = k/N(k = 0, 1, 2, \cdots)$, these states are sufficiently dense for large $N$ in the thermodynamic state space $\Omega$. Therefore, one can
obtain all the thermodynamic properties of the system. In fact, using Eq. (64), we have [78]
\[ \frac{\partial x_{N,0}}{\partial \kappa_0} = \frac{2}{(1-x_{N,0}) \partial \beta / \partial x_0 - \beta} + o(N^0) = O(N^0). \] (77)
Therefore,
\[ x_{N,0}^\eta ((k+1)/N) - x_{N,0}^\eta (k/N) = O(N^{-1}), \] (78)
which implies \( x_{N,0}^\eta \) is dense in the thermodynamic limit.

E. Summary of Parameter Dependence

To summarize this section, although the parameter \( \kappa \) of the SE is not directly related to familiar thermodynamic quantities, such as the intensive parameter, it corresponds to a point in the thermodynamic state space, and, by varying it, we can investigate the properties of a series of equilibrium states. In particular, by simply computing the thermodynamic function given by the SE as a function of \( \kappa \), one can obtain all the thermodynamic properties of the system. As compared with the conventional generalized ensembles, it is easier to compute statistical-mechanical quantities while varying conventional generalized ensembles, it is easier to compute statistical-mechanical quantities while varying \( \kappa \) because the SE allows a much wider choice of the function \( \eta \).

VIII. USAGE OF THE SE

Let us explain how to use the SE when applying it to concrete calculations.

First, choose \( \eta \) which satisfies conditions [A]-[D] depending on the physical situations and the numerical method to be used. To obtain accurate results, special attention should be paid to condition [B]. When one can deal with the thermodynamic limit, it is sufficient if \( s_{TD}(x) - \eta(\kappa; x) \) is strongly concave as required by condition [B]. However, in practical calculations for finite \( N \) that is not so large, it is necessary to take the convexity of \( \eta \) strong enough such that it overcomes the concavity breaking caused by finite-size effects [29].

Next, construct the SE associated with \( \eta \) chosen above according to Eq. (23) and (24). Then, the density matrix \( \rho_N^\eta \) always gives a macroscopically definite equilibrium state. Therefore, by calculating the expectation values in the density matrix, one can obtain the equilibrium values of the local observables and additive observables for any equilibrium state in the thermodynamic state space, including the first-order phase transition regions.

One can also calculate genuine thermodynamic quantities of the equilibrium state. In particular, using Eq. (64), one can obtain the intensive parameters just by calculating the expectation value of \( \hat{x}_N \), without resorting to numerical differentiation.

Furthermore, one can obtain other genuine thermodynamic quantities, such as the thermodynamic entropy density \( s_{TD} \), by using Eqs. (63) or (71). In particular, by using Eq. (71), one can obtain all the thermodynamic properties of the system by simply computing \( \psi_N^\eta \) as a function of \( \kappa \).

In the above manner, one can fully investigate microscopic structures and thermodynamic properties of general quantum systems, even for phase coexistence states without any ad hoc procedures such as finding and imposing clever boundary conditions according to the phases to be coexisted. We will demonstrate this point in Section IX.

IX. FREE SPINS

In this and next sections, we apply our formulation to concrete examples and demonstrate its validity and availability. As the first example, we apply our formulation to the free spins, which was mentioned in Section III in this section. Although this system does not undergo a first-order phase transition, it will help to understand properties of the SE with noncommutative \( \hat{x}_N \).

A. Comparison with the canonical ensemble

As discussed in Section II.C, the CE always gives the correct thermodynamic functions. Furthermore, in this simple model the CE also gives the correct equilibrium state because the phase transition does not occur. By contrast, as discussed in Section III, we cannot employ either the MCE or the RE to the free spin model defined by Eqs. (14) and (15) because \( \hat{X}_{N,0} \) and \( \hat{X}_{N,1} \) do not commute. Let us confirm that the SE gives the correct equilibrium state and thermodynamic functions even in this case by comparing them with those obtained from the CE.

We have a wide choice of the parameter space \( K \) of \( \kappa \) and the functional form of \( \eta \). We here choose them as
\[ K = (0, \infty) \times \Re, \] (79)
\[ \eta(\kappa; x) = \kappa_0 x_0 + \frac{1}{2} \lambda (x_1 - \kappa_1)^2, \] (80)
where \( \lambda \) is a positive constant. Since this \( \eta \) satisfies all conditions [A]-[D] this is an SE, and therefore \( \hat{x}_N \) has a macroscopically definite value in its density matrix, as shown in Eq. (62).

On the other hand, the CE for this system is obtained by taking \( \eta \) as Eq. (65), i.e.,
\[ c(\pi; x) = \pi_0 x_0 + \pi_1 x_1. \] (81)
This \( \eta \) for the CE also satisfies conditions [A]-[D] in this simple system because a first-order phase transition is absent. Hence, \( \hat{x}_N \) has a macroscopically definite value also in the density matrix of the CE. Therefore, if one takes the values of \( \kappa \) and \( \pi \) appropriately (as Eq. (83) below), the CE and the SE represent the same equilibrium state.
That is, the SE associated with $\eta$ in Eq. [80] is equivalent to the CE not only for the thermodynamic function but also for the density matrix, in the thermodynamic limit.

We demonstrate these facts numerically. In numerical calculations, analytic results are used for the CE. For the SE, we use the thermal pure quantum formulation [77, 79], in which $\hat{\rho}_N^\eta(\kappa)$ is replaced with the (unnormalized) pure state,

$$e^{-N\eta(\kappa; \hat{x}_N)/2} |\psi_{\text{rand}}\rangle,$$  \hspace{1cm} (82)

which gives the same results as $\hat{\rho}_N^\eta(\kappa)$ and $\psi_N^\eta(\kappa)$ with exponentially small probability of errors. Here, $|\psi_{\text{rand}}\rangle$ is a Haar-random vector in the whole Hilbert space. Note that this replacement is valid not only for the above $\eta$ but also for all SEs.

### B. Density Matrix

First, we demonstrate that the density matrix $\hat{\rho}_N^\eta$ given by the SE describes the equilibrium state which has the intensive parameters given by Eq. [64].

Since this model does not undergo the first-order phase transition, the equilibrium state is uniquely specified by the set of intensive parameters $\Pi$. Therefore, in order for the CE and the SE to describe the same equilibrium state in the thermodynamic limit, we choose the parameters $\pi$ and $\kappa$ so that

$$\lim_{N \to \infty} \Pi_N^\pi(\pi) = \lim_{N \to \infty} \Pi_N^\eta(\eta).$$ \hspace{1cm} (83)

In concrete calculations, we fix $\kappa$ and calculate statistical-mechanical quantities in the SE, including $\Pi_N^\eta(\kappa)$. Then we set $\pi$ in such a way that $\pi = \Pi_N^\eta(\kappa)$ for each $N$. By doing so, we have

$$\Pi_N^\pi(\pi = \Pi_N^\eta(\kappa)) = \Pi_N^\eta(\kappa)$$ \hspace{1cm} (84)

from Eq. (66). Therefore, the CE and the SE should describe the same equilibrium state in the thermodynamic limit.

To demonstrate the equivalence for the density matrix, we have plotted in Fig. 1 the $N$ dependence of the difference in the expectation value of $\hat{x}_{N,1} = \frac{1}{N} \sum_{i=1}^{N} \hat{\sigma}_i^y$ between the density matrices given by the CE and the SE,

$$\left| x^\eta_{N,1}(\kappa) - x^\pi_{N,1}(\Pi_N^\eta(\kappa)) \right|. \hspace{1cm} (85)$$

We find that the difference decreases with increasing $N$, proportionally to $N^{-1}$. We thus confirm that the SE gives the same expectation value in the thermodynamic limit.

In addition, we have plotted in Fig. 2 the $N$ dependence of the variances of $\hat{x}_{N,0}$ and $\hat{x}_{N,1}$ in the SE. We find that the variances decay as $O(N^{-1})$. This is consistent with the results obtained by Laplace’s approximation (see Section V A). Therefore, it is confirmed that the SE gives the macroscopically definite state even for the noncommutative case. This is in sharp contrast with the RE, for which the variance of $\hat{x}_{N,0}$ remains finite even in the thermodynamic limit due to the noncommutativity of $\hat{x}_{N,0}$ and $\hat{x}_{N,1}$, as discussed in Section VIB.

These results demonstrate that the SE successfully gives the correct equilibrium state even for systems with noncommutative additive observables.

### C. Thermodynamic function

Next, we demonstrate that the thermodynamic function $\psi^\eta(\kappa)$ of the SE is equivalent to the thermodynamic
entropy via Eqs. (70)-(71).

The free spin model defined by Eqs. 14 and 15 has the normal property that the canonical thermodynamic function \( \psi^c(\pi) \) is equivalent to the thermodynamic entropy:

\[
s_{TD}(x) = \inf_{\pi \in \mathbb{R}^2} \{ \pi \cdot x - \psi^c(\pi) \}.
\]

According to Eq. (70), this \( s_{TD} \) is equivalent to the thermodynamic function \( \psi^\eta(\kappa) \) of the SE:

\[
\psi^\eta(\kappa) = \inf_{x \in \Omega} \{ \eta(\kappa; x) - s_{TD}(x) \}.
\]

To demonstrate this equivalence, we have plotted in Fig. 3 the \( N \) dependence of

\[
\left| \psi^\eta_N(\kappa) - \inf_{x \in \Omega} \{ \eta(\kappa; x) - s_{TD}(x) \} \right|,
\]

where \( s_{TD}(x) \) is calculated from the canonical thermodynamic function using Eq. (86). We find that the difference decreases with increasing \( N \), nearly proportionally to \( N^{-1} \). Therefore, it is confirmed that \( \psi^\eta(\kappa) \) is equivalent to the thermodynamic entropy density in the thermodynamic limit.

X. APPLICATION TO THE TWO-DIMENSIONAL TRANSVERSE FIELD ISING MODEL

We apply our formulation to a system which undergoes a first-order phase transition with an order parameter that does not commute with the Hamiltonian and thereby demonstrate numerically that the SE indeed gives the density matrix corresponding to a phase coexistence state even in such a case which cannot be treated by conventional ensembles.

To be concrete, we apply our formulation to the two-dimensional transverse field Ising model on the square lattice, defined by the Hamiltonian

\[
\hat{H}_N = \hat{X}_{N,0} = -J \sum_{(i,j)} \hat{\sigma}^x_i \hat{\sigma}^x_j - g \sum_{i} \hat{\sigma}^z_i.
\]

Here, \( \langle i, j \rangle \) denotes the nearest neighbor sites \( i \) and \( j \).

We take the coupling \( J \) positive and measure energy in units of \( J \).

A. Inapplicability of conventional ensembles

This model has an ordered phase for small \( g \) and large \( \beta (= \Pi_0) \) [80,86]. Its order parameter is given by

\[
\hat{X}_{N,1} = \sum_i \hat{\sigma}^z_i,
\]

and its conjugate field is the \( z \)-component of a magnetic field, \( f_1 = -\Pi_1/\Pi_0 \) (which should not be confused with the \( x \)-component, \( g \)). As \( f_1 \) is changed, while temperature is fixed at a value lower than the critical temperature, a first-order phase transition occurs at \( f_1 = 0 \). There, \( x_1 \) changes discontinuously as a function of \( f_1 \). (This is called the magnetic-field-driven transition as opposed to the temperature-driven transition.) This indicates that phase coexistence states are realized at \( f_1 = 0 \), and the proportions of different phases cannot be specified by \( f_1 \). Consequently, the CE

\[
\rho^\eta_N \propto \exp[-\beta(\hat{H}_N - f_1 \hat{X}_{N,1})] \tag{91}
\]

cannot give the phase coexistence states (unless some trick such as an artificial boundary condition is used), as discussed in Section III.

In order to obtain phase coexistence states it is necessary to employ an ensemble with macroscopically well-defined order parameter. However, neither the MCE nor the RE is applicable because \( \hat{H}_N \) and \( \hat{X}_{N,1} \) do not commute with each other when \( g \neq 0 \), as pointed out in Section III.

We will show in Section XI C that the SE solves this fundamental problem and successfully describes the first-order phase transition. We also show in Section XI B that the SE has advantages even when this fundamental problem is absent (i.e., when \( g = 0 \)).

B. Zero transverse field

We first consider the case of \( g = 0 \), in which the model reduces to the classical Ising model and hence the fundamental problem mentioned above is absent. We will show that the SE is advantages over the CE even in this case.
1. Methods

We choose the parameter space $K$ of $\kappa$ and $\eta$ as

$$K = (0, \infty) \times \mathbb{R},$$

$$\eta(\kappa; x) = \kappa_0 x + \frac{1}{2} \lambda(x_1 - \kappa_1)^2,$$

where $\lambda$ is a positive constant. As will be described below, this choice of $\eta$ is convenient for classical systems which undergo first-order phase transitions.

In order for the order parameter $x_1$ to have a definite value, the convexity of $\eta$ as a function of $x_1$ must be strong enough. This condition is particularly important for finite systems. In the analysis in Section V, we have used the fact that $\sigma_N - \eta$ can be approximated by the strongly concave function $s_{TD} - \eta$ in the thermodynamic limit. However, in finite systems the concavity of the microcanonical entropy $\sigma_N$ is broken near the first-order phase transition region due to finite-size effects [87, 88]. Therefore, if the convexity of $\eta$ is weak, $\sigma_N - \eta$ can be a nonconcave function for finite $N$, and the analysis using Laplace’s approximation breaks down. To overcome such finite-size effects, we take the convexity of $\eta$ strong enough. Since the second order derivative of $\eta$ with respect to $x_1$ is $\lambda$, the strength of the convexity of $\eta$ can be freely adjusted by tuning the value of $\lambda$. That is, for sufficiently large $\lambda$, $\sigma_N - \eta$ becomes strongly concave, and the order parameter has a definite value. In fact, Eq. (31) gives

$$\text{Tr}[\hat{x}_{N,1}^2] = N^{-1} \left[ \lambda - \frac{\partial^2 s_{TD}}{\partial x_1^2} (x_\text{max}^\eta) + \left( \frac{\partial^2 s_{TD}}{\partial x_0^2} (x_\text{max}^\eta) \right)^2 \right]^{-1} + o(N^{-1}),$$

Therefore, the variance of $\hat{x}_{N,1}$ scales as $O(N^{-1}\lambda^{-1})$ for sufficiently large $N$ and $\lambda$.

From Eq. (64), the inverse temperature $\beta = \Pi_0$ is given directly by $\kappa_0$ as

$$\beta_N^\eta = \Pi_{N,0}^\eta = \kappa_0.$$

Equation (64) also gives the intensive parameter conjugate to $X_1$ as

$$\Pi_{N,1}^\eta = \lambda(x_{N,1}^\eta - \kappa_1),$$

which can easily be calculated from the expectation value $x_{N,1}^\eta$. By combining this with Eq. (95), we can calculate the magnetic field conjugate to the order parameter as

$$f_{N,1}^\eta = -\frac{\lambda(x_{N,1}^\eta - \kappa_1)}{\kappa_0}.$$

Using these formulas, one obtains the intensive parameters without differentiating the thermodynamic functions numerically.

We calculate the statistical-mechanical quantities in the SE using the replica exchange Monte Carlo calculations [89], in which the acceptance probability can be easily computed using the Metropolis algorithm [90] in almost the same manner as in the CE. In the SE, the equilibrium state changes continuously in $\kappa$ even in the phase transition region, as explained in Section VII. Therefore, the exchange of configurations between adjacent replicas is accepted with high probability, and the replica exchange method works well (as in the case of the ensembles with macroscopically well-defined internal energy in the temperature-driven first-order phase transition region [91, 92]). By contrast, in the CE, different phases are separated by the free energy barrier [92] and the equilibrium state changes discontinuously in the parameters of the ensemble. This greatly degrades the performance of the replica exchange method in the CE.

In the SE, boundary conditions can be imposed arbitrarily because the order parameter has a definite value without imposing artificial boundary conditions. In the present numerical simulations, we employ periodic boundary conditions. Owing to this choice, we can eliminate surface effects, which are of the same order as the effects of the phase interfaces. That is, the SE enables us to study the phase interfaces without suffering from the surface effects.

2. Results

We have plotted in Fig. 4 the $N$ dependence of the variances of $\hat{x}_{N,1}$ in the CE and in the SE. In order to compare them in the first-order phase transition region where $\beta > \frac{1}{2} \log(1 + \sqrt{2}) \approx 0.44$ and $f_1 = 0$, we focus on the equilibrium state with $\beta = 0.45$ and $f_1 = 0$. Accordingly, we take $\kappa = (0.45, 0)$ so that $\beta_N^\eta = 0.45$ and $f_{N,1}^\eta = 0$ from Eqs. (95) and (96).

It is seen that in the case of the CE the variance remains finite even in the thermodynamic limit. This implies that the CE gives a statistical mixture of macroscopically distinct states which have the same values of the intensive parameters. In fact, as shown in the upper insets of Fig. 4, there are two typical spin configurations for the CE, which are macroscopically homogeneous states (i.e., single phases) with positive or negative $x_1$.

By contrast, in the case of the SE, the variance vanishes in the thermodynamic limit as $O(N^{-1})$. This implies that the SE successfully gives a phase coexistence state, as can be seen from the lower insets of Fig. 4. We have thus confirmed that the SE is a microcanonical-like ensemble and gives the phase coexistence state.

In order to illustrate how the convexity of $\eta$ controls the variance of $\hat{x}_{N,1}$, we have plotted the variance as a function of $\lambda$ in Fig. 5. It is seen that the variance becomes smaller as the convexity of $\eta$ becomes stronger. This is consistent with the analytical result of Eq. (94).

To see more details, we have plotted in Fig. 6 the relation between the magnetic field $f_{N,1}^\eta$ and the order pa-
FIG. 4. \(N\) dependence of the variances of \(\hat{x}_{N,1}\) in the CE and in the SE associated with \(\eta\) in Eq. (93) at a first-order phase transition point (\(\beta = 0.45\) and \(f_1 = 0\)) of the two-dimensional classical Ising model. Insets show typical snapshots of the Monte Carlo simulations (white represents \(\langle \hat{\sigma}_z^i \rangle = +1\) and black represents \(\langle \hat{\sigma}_z^i \rangle = -1\)). Two snapshots are shown for each ensemble.

\[
\text{Tr}\left[(\hat{x}_{N,1} - x_{N,1})^2\hat{\rho}_N\right] \propto N^{-1}
\]

FIG. 5. Relation between the strength \(\lambda\) of the convexity of \(\eta\) defined by Eq. (93) and the variance of \(\hat{x}_{N,1}\) in the SE at the first-order phase transition point (\(\beta = 0.45\) and \(f_1 = 0\)) of the two-dimensional classical Ising model with \(N = 32^2\) spins.

\[
\text{Tr}\left[(\hat{x}_{N,1} - x_{N,1}^\eta)^2\hat{\rho}_N\right] \propto \lambda^{-1}
\]

C. Finite transverse field

To demonstrate that the SE gives phase coexistence states with an order parameter noncommutative with the Hamiltonian, we consider the case of \(g \neq 0\) and take a moderate value, \(g = 1\).

Parameter \(x_{N,1}^\eta\), in the ordered phase for the CE and for the SEs with various values of \(\lambda\). Again, we take \(\kappa_0 = 0.45\).

When the CE is used, \(x_{N,1}^\eta = \text{Tr}[\hat{x}_{N,1}\hat{\rho}_N]\) cannot be a multivalued function of \(f_1\) (because the CE is a function of \(f_1\)) and hence varies monotonically and continuously. The singularities of thermodynamic functions in the first-order phase transition region are almost smeared out due to the large fluctuation inherent in the CE in such a region. This makes it difficult to identify the phase transition and to determine its order [38, 93, 94].

It is thus confirmed that thermodynamic anomalies are correctly obtained and the phase transition can be detected directly by the SE.

It is also seen from Fig. 6 that the results of the SE become insensitive to the magnitude of \(\lambda\) for sufficiently large \(\lambda\) (\(\gtrsim 1\)). Therefore, one can use an arbitrary value of \(\lambda\) as long as it is sufficiently large. This is understood from the derivation in Section V: As long as \(\sigma_N - \eta\) is well approximated by the strongly concave function \(s_{TD} - \eta\), the probability distribution \(p_N^\eta\) has a sharp peak, and the statistical-mechanical quantities do not depend on the details of \(\eta\).

We have thus confirmed that by using the SE one can obtain phase coexistence states and finite-size effects due to phase interfaces for the commutative case. These results also demonstrate that Laplace’s approximation used in Section V will become exact in the thermodynamic limit.
1. Methods

We choose the parameter space \( K \) of \( \kappa \) and \( \eta \) as
\[
K = (0, +\infty) \times (-\infty, +\infty),
\]
\[
\eta(\kappa; x) = \kappa_0 x_0 + \kappa_1 x_1 - 2\nu \log(x_1 + 1),
\]
where \( \nu \) is an appropriate positive constant (see below).

This choice of \( \eta \) is particularly convenient for quantum systems which undergo a first-order phase transition because, as shown in Appendix C, the density matrix can be approximated as the product of local operators, and therefore the SE can be numerically constructed easily even for quantum systems.

Since the second order derivative of \( \eta \) with respect to \( x_1 \) is \( 2\nu/(x_1 + 1)^2 \), the strength of the convexity of \( \eta \) can be freely adjusted by tuning the value of \( \nu \). That is, by taking sufficiently large \( \nu \), we can make the order parameter to have a definite value even in the first-order phase transition region.

From Eq. (64), the inverse temperature \( \beta = \Pi_0 \) is given directly by \( \kappa_0 \) as
\[
\Pi_{N,0}^2 = \kappa_0.
\]
Therefore, we can investigate properties of the equilibrium states of inverse temperature \( \beta \) by taking \( \kappa_0 = \beta \). Furthermore, again using Eq. (64), the intensive parameter conjugate to \( X_1 \) can also be easily calculated from the expectation value \( x_{N,1}^0 \) as
\[
\Pi_{N,1}^2 = \kappa_1 - \frac{2\nu}{x_{N,1}^0 + 1}.
\]
Therefore, by combining this with Eq. (100), the magnetic field conjugate to the order parameter can be calculated as
\[
f_{N,1}^\eta = -\frac{\kappa_1 - \frac{2\nu}{x_{N,1}^0 + 1}}{\kappa_0}.
\]

We calculate statistical-mechanical quantities in the SE using the minimally entangled typical thermal states (METTS) algorithm [95, 96], by extending it to the SE using the minimally entangled typical thermal states (METTS) algorithm [95, 96], by extending it to the SE as follows. We take the quantization axis along \( z \)-direction. Then the “classical product states” (product of spin eigenstates along the quantization axis) is
\[
|s\rangle \equiv \bigotimes_i |s_i\rangle \quad (\hat{\sigma}_z^i |s_i\rangle = s_i |s_i\rangle).
\]
We define the METTS of the SE as
\[
|s; \eta\rangle \equiv \frac{1}{\sqrt{\langle s | e^{-N\eta(\hat{X}_N)} | s \rangle}} e^{-\frac{1}{2}N\eta(\hat{X}_N)} |s\rangle.
\]
Using the completeness of the classical product states, we can decompose \( \hat{\rho}_N^\eta \) into a convex mixture of \( |s; \eta\rangle \) as
\[
\hat{\rho}_N^\eta \propto \sum_{s_i = \pm 1} p(s; \eta) |s; \eta\rangle \langle s; \eta|,
\]
where the weight \( p(s; \eta) \) is given by
\[
p(s; \eta) \equiv \langle s | e^{-N\eta(\hat{X}_N)} | s \rangle.
\]

Therefore, the expectation value in \( \hat{\rho}_N^\eta \) can be calculated by averaging the expectation value in \( |s; \eta\rangle \), which is sampled according to the weight \( p(s; \eta) \).

The numerical simulations are performed for the square lattice of size \( L_1 \times L_2 \) with periodic boundary conditions along \( L_1 \)-direction and open boundary conditions along \( L_2 \)-direction.

2. Results

Figure 7 shows the histogram of the number of samples as a function of \( \langle s; \eta| \hat{X}_{N,1} | s; \eta\rangle \) for the CE and the SE. In order to compare them in the first-order phase transition region, where \( \beta \gtrsim 2.15^{-1} \) and \( f_1 = 0 \) [82, 85], we focus on the equilibrium state with \( \beta = 0.5 \) and \( f_1 = 0 \). Hence, we take \( \kappa_0 = 0.5 \) so that \( \beta_0^\eta = 0.5 \) from Eq. (100). Furthermore, we take \( \kappa_1 = 2\nu \). Then, from Eq. (101), the SE gives the density matrix where the order parameter \( x_1 \rightarrow 0 \) in the thermodynamic limit. That is, we study the equilibrium state with \( \beta = 0.5 \) and \( x_1 = 0 \).

For the CE, the histogram of Fig. 7 shows a double peak structure. This implies that the density matrix given by the CE is a statistical mixture of two single-phase states which have the same values of the intensive parameters. To see this more directly, we examined order parameter profiles. Considering that the order parameter \( \hat{X}_{N,i} \) is the sum of \( \hat{\sigma}_z^i \), we have calculated the expectation value of \( \hat{\sigma}_z^i \) of individual lattice sites in typical samples of METTS and have displayed them for two samples in Fig. 8 (left). It is seen that typical METTS of the CE have macroscopically homogeneous profiles of the order parameter, with positive or negative \( x_1 \).

In the SE, by contrast, Fig. 7 shows that the order parameter has a macroscopically definite value. This implies that the SE successfully gives a phase coexistence state. In fact, as shown in Fig. 8 (right), two phases coexist in both samples of the SE. In addition, since the order parameter profile is different between these samples, it is seen that the SE is a convex mixture of the states which are macroscopically identical except for the spatial arrangement of the coexisting phases. As known from thermodynamics, the spatial arrangement of the coexisting phases is not determined by the values of the additive quantities (of the total system) alone. Therefore, the SE is consistent with thermodynamics.

Figure 9 shows the relation between the magnetic field and the order parameter. In the SE, it is seen that \( x_{N,1}^\eta \) is a multivalued function of \( f_{N,1}^\eta \), as in the classical case \( g = 0 \), Fig. 6 (Note that only the upper half region, in which \( x_{N,1}^\eta \geq 0 \), is plotted in Fig. 6) This behavior is due to the presence of interfaces (domain walls) separating the coexisting phases, which are clearly observed in Fig. 8 (right) [106, 29]. In the CE, by contrast, it is a monotonous and continuous function.
FIG. 7. Histogram of the number of samples as a function of $\langle s; \eta | \hat{x}_{N,1} | s; \eta \rangle$ at the first-order phase transition point ($\beta = 0.5$ and $f_1 = 0$) of the two-dimensional transverse field Ising model ($g = 1$) with $L_1 = 5, L_2 = 16$ for the CE and the SE associated with $\eta$ in Eq. (99).

FIG. 8. Order parameter profiles in typical samples of METTS of the CE (left) and the SE (right) associated with $\eta$ in Eq. (99) at the first-order phase transition point ($\beta = 0.5$ and $f_1 = 0$) of the two-dimensional transverse field Ising model ($g = 1$) with $L_1 = 5, L_2 = 16$ (color map, where yellow represents $\langle \hat{\sigma} \rangle^z_i = +1$ and black represents $\langle \hat{\sigma} \rangle^z_i = -1$). Two samples are shown for each ensemble.

These results demonstrate that the SE successfully gives a phase coexistence state with phase interfaces, whereas the CE gives a convex mixture of single-phase states.

XI. SUMMARY AND DISCUSSION

We have extended a generalized ensemble, which we call the squeezed ensemble (SE), in such a way that it is applicable to equilibrium states specified by noncommutative additive observables.

In contrast to the canonical ensemble, additive observables which specify the equilibrium state always have macroscopically definite values in the SE. Furthermore, unlike the microcanonical and the restricted ensembles, the SE is well-defined and well-behaved even when the order parameter(s) does not commute with the other additive observables such as the Hamiltonian. Therefore, it solves the fundamental problems faced by conventional ensembles in studying such quantum systems when they exhibit first-order phase transitions.

Various ensembles are included in the class of the SE. One can choose an appropriate SE depending on the purpose, such as one that is easy to construct. In addition, good analytic properties of the the SE yield practical formulas for thermodynamic quantities such as the entropy and the intensive parameter. For these reasons, the SE is convenient for practical calculations. We have thus established, for the first time, a concrete method for constructing phase coexistence states of general quantum systems.

As an demonstration, we have applied our formulation to the two-dimensional transverse field Ising model at finite temperature, whose order parameter does not commute with the Hamiltonian. We have confirmed that the SE is composed of thermodynamically identical states with large domains (ordered phases) separated by interfaces (domain walls). In addition, we have obtained thermodynamic anomalies peculiar to such phase coexistence states in finite systems. These results demonstrate that the SE successfully gives a phase coexistence state. From a viewpoint of applications to engineering, we expect that the SE enables the incorporation of quantum effects into the analysis and design of materials with phase interfaces.
In this paper, we have formulated the statistical mechanics only for the leading terms of statistical mechanical quantities in the thermodynamic limit for the case where the additive observables do not commute with each other. However, finite-size effects due to phase interfaces, such as the negative susceptibility, are also important properties of phase coexistence states. From the numerical results, for the equilibrium state without phase interfaces, it is expected that finite-size effects on statistical-mechanical quantities of $O(N^0)$ given by the SE is generally $O(N^{-1})$. Therefore, the ensemble dependence, which is also a finite-size effect, should be $O(N^{-1})$. Now let us assume that this also holds for equilibrium states with phase interfaces. Then, since the spatial dimension $\nu$ is larger than 1 for systems that exhibit first-order phase transitions, the finite-size effects of $O(N^{-1/\nu})$, which includes the effects of the phase interfaces, are independent of the ensemble and are expected to be physical. Therefore, it is expected that the SE can correctly give the finite-size effects due to the phase interfaces. A more detailed analysis of the finite-size effects of the SE is left for future work.

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**Appendix A: Derivation of Eq. (18)**

We first calculate the “partition function” of the RE. The projection operator $\hat{P}_N$ can be written as

$$
\hat{P}_N = \sum_{M=M^-}^{M^+} \sum_{s_i=M^-}^{N} \otimes |s_i\rangle \langle s_i| \quad (\hat{\sigma}_i^y |s_i\rangle = s_i |s_i\rangle),
$$

(A1)

where $M^+ \equiv 2[Nm^+/2], M^- \equiv 2[Nm^-/2]$. Therefore, we have

$$
\text{Tr} \left[ \hat{P}_N e^{-\pi_1 \hat{x}_{N,1}} \hat{P}_N \right] = 2^N \cosh^N \pi_1 \sum_{M=M^-}^{M^+} \left( \frac{N}{N+M} \right).
$$

(A2)

Next, we evaluate the expectation value of $\hat{x}_{N,1}$ in $\hat{\rho}_N$. Without loss of generality, we assume $\pi_1 < 0$. Then

$$
\langle 0 | \text{Tr} \left[ \sigma_i^x \hat{P}_N e^{-\pi_1 \hat{x}_{N,1}} \hat{P}_N \right] | 0 \rangle
$$

$$
= -2^N \sinh \pi_1 \cosh^{N-1} \pi_1 \left( \sum_{M=M^-}^{M^+} \left( \frac{N}{N+M} \right)^{M+2} \right) + \left( \frac{N-1}{(N-1)+(M^+1)} \right) \left( \frac{N}{N+M} \right)^{M+1}
$$

$$
= -2^N \sinh \pi_1 \cosh^{N-1} \pi_1 \left( \sum_{M=M^-}^{M^+} \left( \frac{N}{N+M} \right) \right) - N - M^+ \frac{N}{2N} \left( \frac{N}{N+M} \right) - N + M^- \frac{N}{2N} \left( \frac{N}{N+M} \right)
$$

$$
< -2^N \sinh \pi_1 \cosh^{N-1} \pi_1 \left( 1 - \frac{N}{2N} \left( \frac{N}{N+M} \right) \right) \sum_{M=M^-}^{M^+} \left( \frac{N}{N+M} \right)
$$

$$
< -2^N \sinh \pi_1 \cosh^{N-1} \pi_1 (1 - M^-/N) \sum_{M=M^-}^{M^+} \left( \frac{N}{N+M} \right)
$$

(A3)

In the last inequality we have used

$$
\sum_{M=M^-}^{M^+} \left( \frac{N}{N+M} \right) < \left( \frac{N}{N+M} \right)^{M^+M^-} \sum_{n=0}^{M^+M^-} \left( \frac{N}{N+M} \right)^n = \left( \frac{N}{N+M} \right) \left\{ \frac{1}{1 - \frac{M^-}{N+M}} - e^{-\Theta(N)} \right\}.
$$

(A4)

Therefore, using $\lim_{N \to \infty} M^+/N = m^+$, we have

$$
\langle 0 | \lim_{N \to \infty} \text{Tr} \left[ \hat{x}_{N,1} \hat{\rho}_N \right] \leq -(1 - m^-) \tanh \pi_1.
$$

(A5)
Finally, we evaluate the expectation value of $(\hat{x}_{N,1})^2$ in $\hat{\rho}_N$. In the similar manner as above, for any $0 < \epsilon < m^+ - m^-$, we have
\[
\begin{align*}
&\text{Tr} \left[ \sigma^2 \sigma^2 \hat{P}_N e^{-\pi \hat{x}_{N,1} \hat{P}_N} \right] \\
&= 2^N \sinh^2 \pi_1 \cosh^{N-2} \pi_1 \left( 2 \sum_{M=M^-}^{M^+} \left( \frac{N - 2}{2} \left( N - (N-2) + M \right) \right) + \sum_{M=M^-+4}^{M^+} \left( \frac{N - 2}{2} \left( N - (N-2) + (M-2) \right) \right) + \sum_{M=M^-}^{M^+} \left( \frac{N - 2}{2} \left( N - (N-2) + (M+2) \right) \right) \right) \\
&= 2^N \sinh^2 \pi_1 \cosh^{N-2} \pi_1 \left( \sum_{M=M^-}^{M^-+\lfloor N\epsilon \rfloor} \frac{(N + M)(N - M)}{2N(N-1)} \left( \frac{N}{N+M} \right) \right) \\
&> 2^N \sinh^2 \pi_1 \cosh^{N-2} \pi_1 \left( 1 - M^-/N - \epsilon \right) \sum_{M=M^-}^{M^-+\lfloor N\epsilon \rfloor} \left( \frac{N}{N+M} \right) \\
&= 2^N \sinh^2 \pi_1 \cosh^{N-2} \pi_1 \left( 1 - M^-/N - \epsilon - e^{-\Theta(N)} \right) \sum_{M=M^-}^{M^+} \left( \frac{N}{N+M} \right). \quad (A6)
\end{align*}
\]
Therefore, we have
\[
\lim_{N \to \infty} \text{Tr} \left[ (\hat{x}_{N,1})^2 \hat{\rho}_N \right] \geq (1 - m^- - \epsilon) \tanh^2 \pi_1. \quad (A7)
\]
Since the choice of $\epsilon$ was arbitrary, passing to the limit as $\epsilon \to 0$, we obtain
\[
\lim_{N \to \infty} \text{Tr} \left[ (\hat{x}_{N,1})^2 \hat{\rho}_N \right] \geq (1 - m^-) \tanh^2 \pi_1. \quad (A8)
\]

**Appendix B: Proof of Theorem 1**

Using Eq. \[43\] and $\| \hat{x}_{N,i} \| \leq \| \hat{\eta}_i \|( < \infty)$, we have
\[
\lim_{N \to \infty} \| \eta(\hat{x}_N) - \eta(\hat{x}_N) \| = 0. \quad (B1)
\]
That is, for any $\epsilon > 0$, there exists $N_0 \in \mathbb{N}$ such that $\| \eta(\hat{x}_N) - \eta(\hat{x}_N) \| < \epsilon$ for any $N > N_0$. Then it follows that
\[
-\eta(\hat{x}_N) - \epsilon < -\eta(\hat{x}_N) < -\eta(\hat{x}_N) + \epsilon. \quad (B2)
\]
Therefore, by using Weyl’s inequality \[97\], we have
\[
\text{Tr} \left[ e^{-N\eta(\hat{x}_N)} \right] < \text{Tr} \left[ e^{-N\eta(\hat{x}_N)} \right] < \text{Tr} \left[ e^{-N\eta(\hat{x}_N)} + N \epsilon \right]. \quad (B3)
\]
By definition of $\psi_N^\eta$, this implies that
\[
\psi_N^\eta - \epsilon < \psi_N^\eta < \psi_N^\eta + \epsilon. \quad (B4)
\]

**Appendix C: Proof of Theorem 2**

To prove Theorem 2, we first prove the following lemma.
Lemma 1. Let \( \{f_n\}_{n \in \mathbb{N}} \) be a sequence of real-valued differentiable functions on \( I \) such that \( \{f_n(x_0)\}_{n \in \mathbb{N}} \) is bounded for some \( x_0 \in I \) and \( \{f'_n\}_{n \in \mathbb{N}} \) is uniformly bounded. Then there exists a subsequence \( \{f_{n_k}\}_{k \in \mathbb{N}} \) that converges uniformly on \( I \).

Proof. By the Arzelà-Ascoli theorem \[76\], it is sufficient to show the uniform boundedness and equicontinuity of \( \{f_n\}_{n \in \mathbb{N}} \).

(Uniform boundedness) Uniform boundedness of \( \{f'_n\}_{n \in \mathbb{N}} \) implies by the mean value theorem that for all \( n \in \mathbb{N} \) and \( x, y \in I \),

\[
|f_n(x) - f_n(y)| \leq M|x - y|,
\]

where \( M \equiv \sup_{n \in \mathbb{N}, x \in I} |f'_n(x)| \). In addition, since \( \{f_n(x_0)\}_{n \in \mathbb{N}} \) is bounded, we have, for all \( n \in \mathbb{N} \) and \( x \in I = [a, b] \),

\[
|f_n(x)| \leq F + M|b - a|,
\]

where \( F \equiv \sup_{n \in \mathbb{N}} |f_n(x_0)| \). Therefore, \( \{f_n\}_{n \in \mathbb{N}} \) is uniformly bounded.

(Equicontinuity) Given \( \epsilon > 0 \), let \( \delta \equiv \frac{\epsilon}{M} \). Then, using Eq. (C1), we have

\[
|x - y| < \delta \Rightarrow |f_n(x) - f_n(y)| < \epsilon
\]

for all \( x, y \in I \). Therefore, \( \{f_n\}_{n \in \mathbb{N}} \) is equicontinuous.

\( \square \)

Proof of Theorem 2. Let us introduce the generating functions

\[
\phi_{N}^{\hat{\eta}, \hat{\theta}}(\lambda) \equiv -\frac{1}{N} \log \text{Tr} \left[ e^{-N(\eta(\hat{x}_N) + \lambda \theta(\hat{x}_N))} \right].
\]

Taking the derivative of \( \phi_{N}^{\hat{\eta}, \hat{\theta}} \), we obtain the expectation value of \( \theta(\hat{x}_N) \) in \( \rho_{N}^{\hat{\eta}, \hat{\theta}}(\lambda) \) as

\[
\frac{d\phi_{N}^{\hat{\eta}, \hat{\theta}}}{d\lambda}(\lambda) = \langle \theta(\hat{x}_N) \rangle_{N}^{\hat{\eta}, \hat{\theta}}(\lambda).
\]

In particular, at \( \lambda = 0 \), it coincides with the expectation value in \( \rho_{N}^{\eta} \).

Let \( d \) be the dimension of the local Hilbert space on each site. Then we have

\[
d^{N}e^{-N\|\eta(\hat{x}_N)\|} \leq \text{Tr} \left[ e^{-N\eta(\hat{x}_N)} \right] \leq d^{N}e^{-N\|\eta(\hat{x}_N)\|}.
\]

Therefore, we observe that \( \left\{ \phi_{N}^{\hat{\eta}, \hat{\theta}}(0) \right\}_{N \in \mathbb{N}} \) is bounded. In addition, since \( \frac{d\phi_{N}^{\hat{\eta}, \hat{\theta}}}{d\lambda}(\lambda) = \langle \theta(\hat{x}_N) \rangle_{N}^{\hat{\eta}, \hat{\theta}}(\lambda) \leq \|\theta(\hat{x}_N)\| \),

\[
\left\{ \frac{d\phi_{N}^{\hat{\eta}, \hat{\theta}}}{d\lambda} \right\}_{N \in \mathbb{N}}
\]

is uniformly bounded on any closed and bounded interval. Therefore, by Lemma 1, there exists a subsequence \( \left\{ \phi_{N_k}^{\hat{\eta}, \hat{\theta}} \right\}_{k \in \mathbb{N}} \) that converges (uniformly on compacts in \( \mathbb{R} \)). For this limit, in the same way as in the proof of Theorem 1, it can be shown that

\[
\phi_{\eta, \theta}(\lambda) \equiv \lim_{k \to \infty} \phi_{N_k}^{\hat{\eta}, \hat{\theta}}(\lambda) = \lim_{k \to \infty} \phi_{N_k}^{\eta, \theta}(\lambda)
\]

for all \( \lambda \in \mathbb{R} \).

Since \( \theta(\hat{x}_N) \) commutes with \( \eta(\hat{x}_N) \), we have

\[
\frac{d^2\phi_{N}^{\hat{\eta}, \hat{\theta}}}{d\lambda^2}(\lambda) = -N\text{Tr} \left[ \left( \theta(\hat{x}_N) - \langle \theta(\hat{x}_N) \rangle_{N}^{\hat{\eta}, \hat{\theta}}(\lambda) \right)^2 \rho_{N}^{\hat{\eta}, \hat{\theta}}(\lambda) \right].
\]
Thus, using assumption [ii] we find that \( \left\{ \frac{d^2 \phi_{\eta, \theta}}{d \lambda^2} \right\}_{N \in N} \) is uniformly bounded on \( I \). Hence, by Lemma 1, there exists a subsequence \( \left\{ \frac{d \phi_{\eta, \theta}}{d \lambda} \right\}_{i \in N} \) that converges uniformly on \( I \). Therefore, \( \phi_{\eta, \theta} \) is continuously differentiable on \( I \) and its derivative is given by

\[
\frac{d \phi_{\eta, \theta}}{d \lambda}(\lambda) = \lim_{l \to \infty} \frac{d \phi_{\eta, \theta, N_l}}{d \lambda} = \lim_{l \to \infty} (\hat{x}(\mathbf{x}_{N_l}))_{N_l}^{\eta, \theta} (\lambda)
\]

for all \( \lambda \in I \).

Since \( \phi_{S_{\eta, \theta}} \) is concave, using Griffiths’s lemma, we obtain

\[
\frac{d \phi_{\eta, \theta}}{d \lambda}(\lambda) = \lim_{k \to \infty} \frac{d \phi_{\eta, \theta, N_k}}{d \lambda} = \lim_{k \to \infty} (\hat{x}(\mathbf{x}_{N_k}))_{N_k}^{\eta, \theta} (\lambda).
\]

for all \( \lambda \in I \).

From the above, together with assumption [i] we have

\[
\lim_{N \to \infty} (\hat{x}(\mathbf{x}_{N}))_{N}^{\eta, \theta} (0) = \lim_{l \to \infty} (\hat{x}(\mathbf{x}_{N_l}))_{N_l}^{\eta, \theta} (0) = \lim_{k \to \infty} (\hat{x}(\mathbf{x}_{N_k}))_{N_k}^{\eta, \theta} (0) = \lim_{N \to \infty} (\hat{x}(\mathbf{x}_{N}))_{N}^{\eta, \theta} (0).
\]

\[\square\]

Appendix D: Proof of Properties 1-4

**proof of Property 1.** Using Eq. (59) and letting \( f(x) = x_i \), we get

\[
\lim_{N \to \infty} (\hat{x}_{N,j})_{N}^{\eta, \theta} = x_{\text{max},i}^{\eta, \theta}.
\]

We then apply Theorem 2 with \( \theta = x_i \), and thereby relate this to the expectation value of \( \hat{x}_{N,i} \) in the SE for the noncommutative set \( \hat{x}_N \). To do so, we check the assumptions of the theorem. More specifically, we examine the variance of \( \hat{x}_{N,i} \) in the density matrix

\[
\rho_{\eta, \theta}^{\hat{x}_{N,i}}(\lambda) \propto e^{-N(\eta(\hat{x}_N) + \lambda \theta(\hat{x}_N))},
\]

which is constructed from the commutative set \( x_N \).

First, we show that there exists a bounded closed interval \( I (\ni 0) \) such that for any \( \lambda \in I \), \( \eta + \lambda \theta \) satisfies condition (B). Since we have chosen \( \theta = x_i \), the Hesse matrix \( H[s_{TD} - (\eta + \lambda \theta)](x) \) of \( s_{TD}(x) = (\eta(\mathbb{x}) + \lambda \theta(x)) \) is equal to the Hesse matrix \( H[s_{TD} - \eta](x) \) of \( s_{TD}(x) - \eta(x) \):

\[
H_{kl}[s_{TD} - (\eta + \lambda \theta)](x) = H_{kl}[s_{TD} - \eta](x) = \frac{\partial^2 s_{TD}}{\partial x_k \partial x_l}(x) - \frac{\partial^2 \eta}{\partial x_k \partial x_l}(x).
\]

Since \( \eta \) satisfies condition (B) the Hesse matrix of \( s_{TD} - \eta \) is negative definite in a neighborhood of \( x_{\text{max}}^{\eta, \theta} \). Therefore, the Hesse matrix of \( s_{TD}(x) = (\eta(x) + \lambda \theta(x)) \) is also negative definite in a neighborhood of \( x_{\text{max}}^{\eta, \theta} \). By the implicit function theorem, in a neighborhood of \( \lambda = 0 \), the maximum point \( x_{\text{max}}^{\eta, \theta}(\lambda) \) of \( s_{TD}(x) - (\eta(x) + \lambda \theta(x)) \) changes continuously from \( x_{\text{max}}^{\eta, \theta}(0) \) with respect to \( \lambda \). Therefore, taking \( I (\ni 0) \) narrow enough, for any \( \lambda \in I \), the Hesse matrix of \( s_{TD}(x) - (\eta(x) + \lambda \theta(x)) \) is negative definite in a neighborhood of \( x_{\text{max}}^{\eta, \theta}(\lambda) \). That is, for any \( \lambda \in I \), \( \eta + \lambda \theta \) satisfies condition (B).

Next, for \( I \) taken as above, we show that Eq. (49) of assumption [ii] holds. Let \( H \) be a Hesse Matrix of \( s_{TD}(x) - (\eta(x) + \lambda \theta(x)) \) at \( x_{\text{max}}^{\eta, \theta}(\lambda) \). Since \( \eta + \lambda \theta \) also satisfies condition (B) in the same way as discussed in Section VI.D it can be seen that the probability distribution of \( \hat{x}_N \) in the density matrix \( \rho_{\eta, \theta}^{\hat{x}_{N,i}}(\lambda) \) can be well approximated by the Gaussian distribution with the covariance matrix \( -N^{-1} H^{-1} \). Therefore, we obtain

\[
\text{Tr} \left[ \left( \hat{x}_{N,i} - (\hat{x}_{N,i})_{N}^{\eta, \theta} (\lambda) \right)^2 \rho_{\eta, \theta}^{\hat{x}_{N,i}}(\lambda) \right] = N^{-1} |(H^{-1})_{ii}| + o(N^{-1}).
\]

(4D)
Thus, we see that indeed assumption [ii] of Theorem 2 holds.

From the above, we can apply Theorem 2 and we obtain

\[
\lim_{N \to \infty} \langle \hat{x}_{N,i} \rangle_N^\eta = \lim_{N \to \infty} \langle \hat{x}_{N,i} \rangle_N^\eta = x_{\text{max},i}^\eta.
\]  

(D5)

Therefore, we have Eq. (61).

proof of Property 2. Using Eq. (59) and letting \( f(x) = (x_i)^2 \), we get

\[
\lim_{N \to \infty} \langle (\hat{x}_{N,i})^2 \rangle_N^\eta = (x_{\text{max},i}^\eta)^2.
\]

(D6)

We then apply Theorem 2 with \( \theta = (x_i)^2 \), and thereby relate this to the expectation value of \( (\hat{x}_{N,i})^2 \) in the SE for the noncommutative set \( \hat{x}_N \). To do so, we check the assumptions of the theorem. More specifically, we examine the variance of \( \theta(\hat{x}_{N,i}) = (\hat{x}_{N,i})^2 \) in the density matrix

\[
\rho_{\eta,\lambda}^N(\lambda) \propto e^{-N(\eta(\hat{x}_N) + \lambda \theta(\hat{x}_N))},
\]

which is constructed from the commutative set \( x_N \).

First, we show that there exists a bounded closed interval \( I(\exists 0) \) such that for any \( \lambda \in I, \eta + \lambda \theta \) satisfies condition [B].

Since we have chosen \( \theta = (x_i)^2 \), the Hesse matrix \( H[s_{\text{TD}} - (\eta + \lambda \theta)](x) \) of \( s_{\text{TD}}(x) - (\eta(x) + \lambda \theta(x)) \) is related to the Hesse matrix \( H[s_{\text{TD}} - \eta](x) \) of \( s_{\text{TD}}(x) - \eta(x) \) as

\[
H_{kl}[s_{\text{TD}} - (\eta + \lambda \theta)](x) = H_{kl}[s_{\text{TD}} - \eta](x) - 2\lambda \delta_{ik} \delta_{jl}.
\]

(D8)

Thus, when \( H[s_{\text{TD}} - \eta](x) \) is negative definite, \( H[s_{\text{TD}} - (\eta + \lambda \theta)](x) \) is also negative definite. Since \( \eta \) satisfies condition [B], the Hesse matrix of \( s_{\text{TD}} - \eta \) is negative definite in a neighborhood of \( x_{\text{max}}^\eta \). Therefore, the Hesse matrix of \( s_{\text{TD}}(x) - (\eta(x) + \lambda \theta(x)) \) is also negative definite in a neighborhood of \( x_{\text{max}}^\eta \). By the implicit function theorem, in a neighborhood of \( \lambda = 0 \), the maximum point \( x_{\text{max}}^\eta(\lambda) \) of \( s_{\text{TD}}(x) - (\eta(x) + \lambda \theta(x)) \) changes continuously from \( x_{\text{max}}^\eta \) with respect to \( \lambda \). Therefore, taking \( I = [0, \delta] \) for some positive constant \( \delta \), for any \( \lambda \in I \), the Hesse matrix of \( s_{\text{TD}}(x) - (\eta(x) + \lambda \theta(x)) \) is negative definite in a neighborhood of \( x_{\text{max}}^\eta(\lambda) \). That is, for any \( \lambda \in I, \eta + \lambda \theta \) satisfies condition [B].

Next, for \( I \) taken as above, we show that Eq. (49) of assumption [ii] holds. Let \( H \) be a Hesse Matrix of \( s_{\text{TD}}(x) - (\eta(x) + \lambda \theta(x)) \) at \( x_{\text{max}}^\eta(\lambda) \). Since \( \eta + \lambda \theta \) also satisfies condition [B], in the same way as discussed in Section 2, it can be seen that the probability distribution of \( \hat{x}_N \) in the density matrix \( \rho_{\eta,\lambda}^N(\lambda) \) can be well approximated by the Gaussian distribution with the covariance matrix \( -N^{-1}H^{-1} \). Therefore, denoting \( \delta \hat{x}_{N,i}(\lambda) \equiv \hat{x}_{N,i} - \langle \hat{x}_{N,i} \rangle_N^\eta(\lambda) \), we obtain

\[
\begin{align*}
\text{Tr} \left[ \left( \langle \hat{x}_{N,i} \rangle_N^\eta \right)^2 - \left( \langle \hat{x}_{N,i} \rangle_N^\eta \right)^2 \rho_{\eta,\lambda}^N(\lambda) \right]
&= 4 \left( \langle \hat{x}_{N,i} \rangle_N^\eta(\lambda) \right)^2 \left( \langle \delta \hat{x}_{N,i} \rangle_N^\eta(\lambda) \right)^2 \\
&+ 4 \langle \delta \hat{x}_{N,i} \rangle_N^\eta(\lambda) \left( \langle \delta \hat{x}_{N,i} \rangle_N^\eta(\lambda) \right)^4 \\
&= 4N^{-1} \left( \langle \hat{x}_{N,i} \rangle_N^\eta(\lambda) \right)^2 \left[ (H^{-1})_{ii} \right] + o(N^{-1}).
\end{align*}
\]

(D9)

Thus, we see that indeed assumption [ii] of Theorem 2 holds.

From the above, we can apply Theorem 2 and we obtain

\[
\lim_{N \to \infty} \langle (\hat{x}_{N,i})^2 \rangle_N^\eta = \lim_{N \to \infty} \langle (\hat{x}_{N,i})^2 \rangle_N^\eta = (x_{\text{max},i}^\eta)^2.
\]

(D10)

Therefore, together with Eq. (D5), we have Eq. (62).

proof of Property 3. By using Theorem 1 and Eq. (60), in the thermodynamic limit, we have

\[
\lim_{N \to \infty} \psi_N^\eta = \lim_{N \to \infty} \psi_N^\eta = \eta(\rho_{\text{max}}^\eta) - s_{\text{TD}}(\rho_{\text{max}}^\eta).
\]

(D11)
This, together with Eq. (D5), implies
\[ \eta(x_N^\eta) - \psi_N^\eta = s_{\text{TD}}(x_{\text{max}}^\eta) + o(N^0). \] (D12)

Therefore, we have Eq. (63).

**proof of Property 4.** By using Eq. (28), which is also true for the SE for \( x_N \) as described in Section VI-D, we have
\[ \Pi_i(x_{\text{max}}^\eta) = \partial s_{\text{TD}} / \partial x_i(x_{\text{max}}^\eta). \] (D13)

This, together with Eq. (D5), implies
\[ \frac{\partial \eta}{\partial x_i}(x_N^\eta) = \Pi_i(x_{\text{max}}^\eta) + o(N^0). \] (D14)

Therefore, we have Eq. (64).

**Appendix E: Proof of Property 6**

Using Eq. (70), we have
\[ s_{\text{TD}}(x) \leq \eta(\kappa; x) - \inf_{x' \in \Omega} \{ \eta(\kappa; x') - s_{\text{TD}}(x') \} \]
\[ = \eta(\kappa; x) - \psi^\eta(\kappa) \] (E1)

for all \( \kappa \in K \). Then we have
\[ s_{\text{TD}}(x) \leq \inf_{\kappa \in K} \{ \eta(\kappa; x) - \psi^\eta(\kappa) \}. \] (E2)

On the other hand, using Eq. (70), we have
\[ \inf_{\kappa \in K} \{ \eta(\kappa; x) - \psi^\eta(\kappa) \} \]
\[ \leq \eta(\kappa'; x) - \psi^\eta(\kappa') \]
\[ = \eta(\kappa'; x) - \inf_{x' \in \Omega} \{ \eta(\kappa'; x') - s_{\text{TD}}(x') \} \]
\[ = \eta(\kappa'; x) - \eta(\kappa'; x_{\text{max}}^\eta(\kappa')) + s_{\text{TD}}(x_{\text{max}}^\eta(\kappa')) \] (E3)

for all \( \kappa' \in K \). The condition (D) implies that there exists \( \kappa' \in K \) such that \( x_{\text{max}}^\eta(\kappa') = x \), then it holds
\[ \inf_{\kappa \in K} \{ \eta(\kappa; x) - \psi^\eta(\kappa) \} \leq s_{\text{TD}}(x). \] (E4)

Therefore, we have Eq. (71).

**Appendix F: information-theoretic interpretation of Eq. (64)**

In this section, we give another derivation of the formula for the intensive parameter, Eq. (64). A great advantage of this proof is that it works even in the case where \( \hat{x}_N \) do not commute with each other because it does not rely on the asymptotic approximation.

Suppose that the SE is outside the phase transition region, and the CE
\[ c(\pi; x) = \pi \cdot x \] (F1)

describes the same equilibrium state as the SE in the thermodynamic limit when \( \pi = \hat{\pi} \). In particular, the following holds:
\[ \lim_{N \to \infty} x_N^\eta = \lim_{N \to \infty} x_N^\eta(\hat{\pi}). \] (F2)
Since \( \lim_{N \to \infty} x^c_N(\pi) \) is assumed to be outside the phase transition region, the canonical thermodynamic function \( \psi^c \) is differentiable at \( \tilde{\pi} \), and its derivative at \( \tilde{\pi} \) is given by

\[
\frac{\partial \psi^c}{\partial \pi_i}(\tilde{\pi}) = \lim_{N \to \infty} x^c_N(\pi).
\] (F3)

Therefore, using Eq. (F2), Eq. (64) can be rephrased as

\[
\lim_{N \to \infty} \left( \tilde{\pi}_j - \frac{\partial \eta}{\partial x_j}(x^c_N(\pi)) \right) = 0.
\] (F4)

We derive Eq. (F4) under reasonable conditions.

### 1. Assumptions

Let us measure the distance between the density matrices by the relative entropy

\[
D(\hat{\rho} \parallel \hat{\sigma}) \equiv \text{Tr} [\hat{\rho} \{ \log \hat{\rho} - \log \hat{\sigma} \}] .
\] (F5)

Since the “distance” between \( \hat{\rho}^N_\eta \) and \( \hat{\rho}^N_\pi(\pi) \) is expected to be minimized at \( \pi = \tilde{\pi} \), it is reasonable to assume that

(i) \[
\frac{\partial D(\hat{\rho}^N_\pi(\pi) \parallel \hat{\rho}^N_\eta)}{\partial \pi_i}(\pi = \tilde{\pi}) = o(N).
\] (F6)

Note that a similar condition

\[
\frac{\partial D(\hat{\rho}^N_\eta \parallel \hat{\rho}^N_\pi(\pi))}{\partial \pi_i}(\pi = \tilde{\pi}) = o(N)
\] (F7)

is equivalent to Eq. (F2), which is a necessary condition for \( \hat{\rho}^N_\pi(\pi) \) and \( \hat{\rho}^N_\eta \) to describe the same equilibrium state. Therefore, it seems reasonable to assume Eq. (F6).

In addition, we assume

(ii) \( \hat{\rho}^N_\pi(\pi) \) has normal fluctuations \([99, 100]\):

\[
\langle \delta \hat{x}_{N;i} \cdots \delta \hat{x}_{N;jN} \rangle_N^c(\pi) = O(N^{-n}),
\] (F8)

where \( \langle \cdot \rangle_N^c = \text{Tr} [\cdot \rho^N_\pi] \). Here, for simplicity of notation, we abbreviate \( \langle \cdots (\cdot - \langle \cdot \rangle_N^\eta) \cdots \rangle^\eta_N \) to \( \langle \cdots \delta \cdots \rangle^\eta_N \).

Finally, we assume

(iii) the \( m \times m \) positive-semidefinite matrix

\[
\Delta_{ij} \equiv \lim_{N \to \infty} N \langle \delta \hat{x}_{N;i} \delta \hat{x}_{N;j} \rangle_N^c(\tilde{\pi})
\] (F9)

is invertible,

where \( \langle \cdot ; \cdot \rangle_N^\eta \) denotes a generalization of the Bogoliubov-Duhamel inner product \([101]\):

\[
\langle \hat{A} ; \hat{B} \rangle^\eta_N \equiv \int_0^1 d\nu \langle e^{+\nu N^\eta(\hat{x}_N)} \hat{A}^\dagger e^{-\nu N^\eta(\hat{x}_N)} \hat{B} \rangle^\eta_N.
\] (F10)

The validity of this assumption is explained as follows. Since \( x^c(\tilde{\pi}) \) is assumed to be outside the phase transition region, \( x^c(\pi) \) is analytic and one-to-one in a neighborhood of \( \tilde{\pi} \). Therefore, \( \frac{\partial x^c_j}{\partial \pi_i}(\tilde{\pi}) \) is an invertible matrix. On the other hand, we have

\[
\Delta_{ij} = \lim_{N \to \infty} \frac{\partial x^c_{N,j}}{\partial \pi_i}(\tilde{\pi}).
\] (F11)

It is expected that we can interchange the limit and differentiation except at phase transition points (see Lemma 1) as

\[
\Delta_{ij} = \lim_{N \to \infty} \frac{\partial x^c_{N,j}}{\partial \pi_i}(\tilde{\pi}) = \frac{\partial x^c_j}{\partial \pi_i}(\tilde{\pi}).
\] (F12)

Therefore, \( \Delta_{ij} \) should be invertible.

Note that assumptions (ii)-(iii) are assumptions on the CE, not on the SE.
2. Proof

To prove Eq. (F4), we first prove the following lemma.

**Lemma 2.** If

\[
\langle \delta \hat{x}_{N(i_1)} \cdots \delta \hat{x}_{N(i_m)} \rangle_N^n = O(N^{-n}), \tag{F13}
\]

then

\[
\langle \delta \hat{x}_{N(i_1)} \cdots \delta \hat{x}_{N(i_m)} \rangle_N^n = O(N^{-\frac{m+n}{2}}). \tag{F14}
\]

**Proof.** Applying the Cauchy-Schwarz inequality

\[
|\langle \hat{A}; \hat{B} \rangle_N^n |^2 \leq \langle \hat{A}; \hat{A} \rangle_N^n \langle \hat{B}; \hat{B} \rangle_N^n , \tag{F15}
\]

and Brooks Harris inequality \[102, 103\]

\[
\langle \hat{A}; \hat{A} \rangle_N^n \leq \frac{1}{2} \langle \{ \hat{A}, \hat{A} \} \rangle_N^n , \tag{F16}
\]

we have

\[
\begin{align*}
|\langle \delta \hat{x}_{N(i_1)} \cdots \delta \hat{x}_{N(i_m)} \rangle_N^n |^2 & \leq \frac{1}{4} \langle \{ \delta \hat{x}_{N(i_1)} \cdots \delta \hat{x}_{N(i_m)}, \delta \hat{x}_{N(i_1)} \cdots \delta \hat{x}_{N(i_m)} \} \rangle_N^n \langle \{ \delta \hat{x}_{N(i_1)} \cdots \delta \hat{x}_{N(i_m)}, \delta \hat{x}_{N(i_1)} \cdots \delta \hat{x}_{N(i_m)} \} \rangle_N^n . \tag{F17}
\end{align*}
\]

Therefore, by assumption, we obtain Eq. (F14). \(\square\)

**Proof of Eq. (F4).** By assumption (iii) and Lemma 2, we have

\[
\langle \delta \hat{x}_{N,i} \cdots \delta \hat{x}_{N(j_m)} \rangle_N^c = O(N^{-\frac{m+n}{2}}). \tag{F18}
\]

In addition, since \(\eta\) is a polynomial, expanding in power series around \(x_N^c(\pi)\), \(\eta(\hat{x}_N)\) can be written as a finite sum as

\[
\eta(\hat{x}_N) = \eta(x_N^c(\pi)) + \sum_j \frac{\partial \eta}{\partial x_j}(x_N^c(\pi)) \delta \hat{x}_N, j + \cdots. \tag{F19}
\]

Therefore, using

\[
\frac{\partial D(\hat{\pi}_N(\pi) \parallel \hat{\rho}_N^c)}{\partial \pi_i} = N^2 \langle \delta \pi_i; c(\pi; \hat{x}_N) ; c(\pi; \hat{x}_N) - \eta(\hat{x}_N) \rangle_N^c (\pi), \tag{F20}
\]

we have

\[
\frac{\partial D(\hat{\pi}_N(\pi) \parallel \hat{\rho}_N^c)}{\partial \pi_i} = \sum_j N^2 \left\{ \langle \delta \hat{x}_{N,i} \cdots \delta \hat{x}_{N,j} \rangle_N^c (\pi) \left( \pi_j - \frac{\partial \eta}{\partial x_j}(x_N^c(\pi)) \right) + O(N^{-\frac{m+n}{2}}) \right\} . \tag{F21}
\]

Therefore, assumption (i) can be rewritten as

\[
\sum_j \Delta_{ij} \lim_{N \to \infty} \left( \hat{x}_j - \frac{\partial \eta}{\partial x_j}(x_N^c(\pi)) \right) = 0. \tag{F22}
\]

Hence, by assumption (iii) we obtain Eq. (F4). \(\square\)
FIG. 10. Trotter step dependence of the statistical-mechanical quantity for the one-dimensional transverse field Ising model $(X_{N,0} = -J \sum_1^N \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z - g \sum_1^N \hat{\sigma}_i^x, X_{N,1} = \sum_1^N \hat{\sigma}_i^x)$ in the SE for $N = 50, J = 1, g = 1$ and $\nu = 3.6, \kappa = (1, 5)$.

Appendix G: Numerical implementation of the SE associated with $\eta$ in Eq. (99)

We calculate statistical-mechanical quantities in the SE associated with $\eta$ in Eq. (99) using the METTS algorithm. To obtain the METTS, one needs to apply $e^{-\frac{1}{2} N \eta(\kappa; \hat{x}_N)}$ to a random product state. Choosing $\eta$ as Eq. (99), this can be easily done as follows.

Consider the general case where $\hat{X}_{N,0}$ and $\hat{X}_{N,1}$ can be written as the sum of local observables:

$$\hat{X}_{N,0} = \sum_{i=1}^N \hat{h}_i, \quad \hat{X}_{N,1} = \sum_{i=1}^N \hat{m}_i,$$

where $\hat{h}_i$ and $\hat{m}_i$ are observables located around site $i$. Then it follows that

$$-\frac{1}{2} N \eta(\kappa; \hat{x}_N) = \frac{1}{\delta} \left\{ \sum_{i=1}^N \delta \hat{\gamma}_i + N \nu \delta \log \left( \sum_{i=1}^N \hat{m}_i + N \right) + \sum_{i=1}^N \delta \hat{\gamma}_i \right\} + \text{const.},$$

where $\hat{\gamma}_i \equiv \frac{1}{4}(\kappa_0 \hat{h}_i + \kappa_1 \hat{m}_i)$. Therefore, by using the Trotter-Suzuki formula [104], $e^{-\frac{1}{2} N \eta(\kappa; \hat{x}_N)}$ is decomposed into a product of local operators as

$$e^{-\frac{1}{2} N \eta(\kappa; \hat{x}_N)} \propto e^{\delta \hat{\gamma}_1} \cdots e^{\delta \hat{\gamma}_N} \left( \sum_{i=1}^N \hat{m}_i + N \right)^{N \nu \delta} e^{\delta \hat{\gamma}_1} \cdots e^{\delta \hat{\gamma}_N} + O(\delta^2).$$

Especially when $N \nu \delta$ and $1/\delta$ are both integers, the right hand side of Eq. (G4) can be obtained by simply multiplying the local operators repeatedly. In particular, by choosing $\nu$ so that $N \nu$ is an integer with many divisors, it is possible to extrapolate the statistical-mechanical quantities to $\delta \to 0$ while taking $N \nu \delta$ as an integer, as shown in Fig. 10. Hence, the SE can be numerically constructed easily even for quantum systems.

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The authors do not know systems with short-range interactions which violate this assumption.

In Refs. [105–107], it was proposed to extend the microcanonical entropy (not the density matrix) to quantum systems whose equilibrium states are specified by two noncommutative additive observables.

We write \( f(N) = \Theta(g(N)) \) when \( f \) is bounded both above and below by \( g \) up to a constant factor in the thermodynamic limit. In addition, to emphasize that we are considering the asymptotic behavior as a function of \( N \), we write \( g(N) \) as \( N^0 \) when \( g(N) = 1 \).

We write \( f(N) = o(g(N)) \) when \( f \) is dominated by \( g \) in the thermodynamic limit such that \( \lim_{N \to \infty} f(N)/g(N) = 0 \).

All arguments in Sections V–VII are valid even if \( \eta \) is a power series and not a polynomial, as long as it defines an operator Lipschitz function in the operator norm.

More specifically, we define \( m \)-dimensional interval \( I_n \) as \( I_n \equiv (n_0 \delta_1, (n_0 + 1) \delta_1) \times \cdots \times (n_{m-1} \delta_m, (n_{m-1} + 1) \delta_m) \), where \( n = (n_0, n_1, \ldots, n_{m-1}) \) \( \in \mathbb{Z}^m \) is the labeling of the interval and \( \delta_i = o(N^0) \) is the side length of the interval. Then this gives the direct sum decomposition of \( \mathbb{Z}^n \).

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Even when \( X_{N,\lambda} \) contains a boundary terms, there exists \( \bar{x}_N \) that satisfies Eqs. (13) and (14), because the boundary terms change the operator norm of \( \bar{x}_N \) by only \( O(N^{-1/\lambda}) \).

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We write \( f(N) = O(g(N)) \) when \( f \) is bounded above by \( g \) up to a constant factor \( K \) in the thermodynamic limit such that \( f(N) \leq Kg(N) \) as \( N \to \infty \).

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