

**Boltzmann entropy for quantum field systems**Kyo Yoshida *Division of Physics, Faculty of Pure and Applied Sciences, University of Tsukuba, 1-1-1 Tennoudai, Tsukuba, Ibaraki 305-8571, Japan*

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A way to construct Boltzmann entropy, i.e., the entropy as a function of a microscopic pure state, for quantum field systems is proposed. Operators that shift the field in wave-vector space are used in the construction. By employing an assumption that some terms emerging due to the shift are negligible in the thermodynamic limit, it is shown that, for almost all states in the ensemble of pure states corresponding to a thermodynamic state, the value of the proposed Boltzmann entropy coincides with that of the thermodynamic entropy for the thermodynamic state. For general self-interacting fields, the Boltzmann entropy evolves with time under Hamiltonian dynamics, so that it is capable of characterizing the thermalization of isolated quantum field systems.

DOI: [10.1103/PhysRevA.101.032110](https://doi.org/10.1103/PhysRevA.101.032110)**I. INTRODUCTION**

The statistical mechanics for thermal equilibrium states in classical and quantum systems are well established in the sense that it satisfactorily provides prescription to obtain macroscopic thermodynamic variables, such as entropy  $S$ , Helmholtz free energy  $F$ , and many others, from the Hamiltonian that determines the microscopic and dynamical nature of the system. However, it may be said that the general consensus on its foundations has not been reached.

Regarding the definition of thermal equilibrium in microscopic terms, there are two views, which may be called the *ensamblist view* and the *individualist view*, where we borrowed the terminology from Ref. [1]. In the former view, a system is in thermal equilibrium when it is a mixed state (or an ensemble of states) that is close to the canonical or microcanonical mixed state (or ensemble), whereas in the latter view, a pure state (or a point in phase space) can be in or out of thermal equilibrium depending on the state.

The ensamblist view has traditionally prevailed, presumably because of its concise formalism. Once the canonical, microcanonical, or some other ensemble corresponding to a thermal equilibrium state is defined from the Hamiltonian of the system, all corresponding thermodynamic variables can be derived through suitable statistical calculations with respect to the ensemble. For example, in classical systems, the entropy  $S$  is given by the form of Gibbs entropy  $S = -\int_{\Gamma} dx \rho(x) \ln \rho(x)$  where  $\Gamma$  is the phase space and  $\rho(x)$  is a probability density function on  $\Gamma$  representing the ensemble. In the case of a canonical ensemble with inverse temperature  $\beta := (k_B T)^{-1}$ , where  $k_B$  is the Boltzmann constant, the probability density function is given by  $\rho^{\text{can},\beta}(x) = \exp[-\beta H(x)]/Z(\beta)$  ( $x \in \Gamma$ ) where  $H(x)$  is the Hamiltonian and  $Z(\beta)$  is the partition function. In quantum systems, the ensemble is represented by the density operator  $\rho$ ; for example, the canonical density operator is given by  $\rho^{\text{can}}(\beta) = \exp(-\beta H)/Z(\beta)$  with the Hamiltonian  $H$  being an operator, and the entropy is given by the form of von Neumann entropy  $S = -\text{tr}[\rho \ln \rho]$ .

On the other hand, the individualist view has its basis in the concept of typicality. Consider an ensemble of (pure) states of a large classical or quantum system and a function of state. Here, we say that the function satisfies the typicality with respect to the ensemble if the value of the function is almost same for almost all states in the ensemble. The state is said to be typical when the value of the function is very close to the ensemble average and it is said to be atypical when the value of the function largely deviates from the average. In the individualist view, thermodynamic variables are functions of (pure) states and they are expected to satisfy the typicality with respect to ensembles corresponding to thermal equilibrium, say microcanonical ensembles or canonical ensembles. Then, we may identify the values of the thermodynamic variables at typical states, which we interpret as thermal equilibrium states, with the ensemble average of those. In the individualist view, the physical objects are individual (pure) states and ensembles are just working tools for computing thermodynamic variables efficiently. It is actually shown in Refs. [2–5] that, in a large quantum system, physical quantities associated with a small subsystem satisfy typicality with respect to the microcanonical ensembles of the large system. Thus, the individualist view has been gaining theoretical support.

As far as thermodynamic variables in thermal equilibrium are concerned, all the outcomes are the same for the both views and there may be little practical reason to distinguish between them. Significant difference between the two views emerges in the case of nonequilibrium processes, especially in thermalization in isolated systems. Note that the Gibbs entropy and the von Neumann entropy do not evolve with time under the Hamiltonian dynamics of isolated systems. Therefore, these entropies are not capable of characterizing thermalization. In the individualist view, thermalization can be understood as follows: When a nonequilibrium state, that is, an atypical state, is chosen as the initial state, it would develop with time into thermal states because they are typical in the ensemble, and the system substantially never comes

back to the original nonequilibrium state nor develops into other nonequilibrium states because they are so rare.

Recently, thermalization in isolated macroscopic quantum systems has become a quite active research topic (see, e.g., Ref. [6] and references cited therein). The individualist view plays an important role in the recent studies and there is a growing consensus that the nature of thermodynamic equilibrium states and thermalization can be analyzed through a single typical pure state and its time evolution [7–10]. Rigol, Dunjko, and Olshanii [7] demonstrated that a pure state of an isolated system of hard-core bosons with additional weak nearest-neighbor repulsions on a two-dimensional lattice do thermalize under Hamiltonian dynamics by monitoring relaxation of the central component of the marginal momentum distribution.

From thermodynamic point of view, entropy is the function that characterizes the thermalization processes. It generally increases under adiabatic thermalization processes. So it is of interest to consider the entropy in the individualist view, that is, entropy defined for microscopic state, or (pure) state. It should satisfy typicality and its ensemble average should coincide with the entropy defined for the ensemble, i.e., the Gibbs entropy or the von Neumann entropy. The concept of entropy as a function of microscopic state is originated by Boltzmann and here we call such entropy the Boltzmann entropy. (See, e.g., Ref. [11] for a review of the Boltzmann entropy. See also the introduction of Ref. [12] for a similar use of the terminology of Gibbs and Boltzmann entropy). Boltzmann introduced a decomposition of the phase space into disjoint subregions in the construction of the Boltzmann entropy for classical systems. For quantum systems, the pioneering work on Boltzmann entropy was given by von Neumann [13]. (Hereinafter, Ref. [13] is referred to as VN29. See Ref. [1] for a review of VN29 from a modern perspective). In VN29, the Boltzmann entropy is defined by using the abstract formalism of the decomposition of the total Hilbert space. Although the existence of many appropriate decompositions of the total Hilbert space is guaranteed, the prescription of the appropriate decompositions for specific systems was not given.

The aim of this paper is to construct a Boltzmann entropy, a function of pure states, for quantum systems on a lattice, or systems of quantum field, and to show that it satisfies some properties that are desirable for the entropy. We restrict the system to quantum field in order to give the explicit construction of the Boltzmann entropy. The present study is inspired by the author’s previous work on the construction of entropy as a function of state in classical field systems [14]. Following the previous work, the construction of the Boltzmann entropy is considered in the wave-vector space and operators that shift the field in the wave-vector space are used.

Recently, Šafránek, Deutsch, and Aguirre [15,16] proposed a decomposition of the total Hilbert space based on a coarse-graining in position space to construct a Boltzmann entropy for systems of many quantum particles (hereinafter, Refs. [15,16] are referred to as ŠDA19). Our study shares interest and aim with ŠDA19 to some extent but the two studies developed to construct different types of Boltzmann entropy. Comparison between the two studies is given in Sec. VI. Very recently, there is an attempt to define not  $c$ -number valued but an operator valued Boltzmann entropy in

Ref. [12]. However, we do not expand the scope of this paper to include the operator valued Boltzmann entropy.

This paper is organized as follows: We start with the general formalism of constructing the Boltzmann entropy in Sec. II. We then introduce a normal distribution model for ensemble of pure states in Sec. III. Next, we give the setting of the quantum field systems in Sec. IV. After these preparations, we construct a Boltzmann entropy for the quantum field systems and examine its properties by using the normal distribution model for ensemble of pure states in Sec. V. We conclude with some discussion of the results in Sec. VI.

## II. GENERAL FORMALISM

We first consider the properties that the Boltzmann entropy  $S(\psi)$ , i.e., entropy as a function of (microscopic, pure) state  $\psi$ , should satisfy, if it is formulated, both in classical and quantum systems. Let  $X$  be a set of thermodynamic variables that specifies a thermodynamic equilibrium state. For example,  $X = (U, V, N)$  or  $X = (\beta, V, N)$ , where  $U$  is the internal energy,  $V$  is the volume,  $N$  is the number of particles, and  $\beta$  is the inverse temperature. In conventional statistical mechanics, a thermodynamic equilibrium state is modeled by a probability density function (PDF)  $P(\psi)$  on the phase space  $\Gamma$  for classical systems and a density operator  $\rho$  for quantum systems. In the next section, we introduce a model PDF  $P(\psi)$  on the Hilbert space  $\mathcal{H}$  which corresponds to a given density operator  $\rho$ , so that a thermodynamic equilibrium state  $X$  both in classical and quantum systems can be described by a PDF on the state space, which will be denoted by  $P^{(X)}(\psi)$ . Let the average with respect to  $P^{(X)}(\psi)$  be denoted by

$$\overline{F(\psi)}^{(X)} := \int_{\mathcal{H}} d\psi P^{(X)}(\psi) F(\psi), \quad (1)$$

for an arbitrary function  $F(\psi)$  of the state  $\psi$ . The overline without superscript ( $X$ ) will mean the average with respect to an arbitrary PDF  $P(\psi)$ .

So that the Boltzmann entropy  $S(\psi)$  is consistent with the thermodynamic entropy  $S(X)$  defined for thermodynamic state  $X$ , the following conditions should be required:

(S1) The average of  $S(\psi)$  with respect to  $P^{(X)}(\psi)$  is equal to the thermodynamic entropy  $S(X)$  in the thermodynamic limit, say  $V \rightarrow \infty$ , i.e.,

$$\lim_{V \rightarrow \infty} \frac{\overline{S(\psi)}^{(X)}}{S(X)} = 1. \quad (2)$$

(S2) The deviation from the mean  $\Delta S(\psi) := S(\psi) - \overline{S(\psi)}^{(X)}$  is small in the thermodynamic limit in the sense that

$$\lim_{V \rightarrow \infty} \frac{[\overline{[\Delta S(\psi)]^2}^{(X)}}{[S(X)]^2} = 0. \quad (3)$$

Note that the thermodynamic limits in the above should be taken by fixing the intensive variables such as  $N/V$ ,  $E/V$ , and  $\beta$ . By virtue of the Chebyshev’s inequality, the conditions (S1) and (S2) imply that  $S(\psi)$  is typically almost equal to  $S(X)$  when  $\psi$  is randomly chosen according to the PDF  $P^{(X)}(\psi)$ .

In addition to being consistent with the thermodynamic entropy, it is desirable for the Boltzmann entropy  $S(\psi)$  to have some properties characterizing nonequilibrium states

and processes. Let  $\psi(t)$  denote the time evolution of the state with respect to the Hamiltonian  $H$  and the initial condition  $\psi(t = 0) = \psi$ . If  $S(\psi)$  is substantially smaller than  $S(X)$  and  $S(\psi(t))$  approaches  $S(X)$  as  $t \rightarrow \infty$ , then we may interpret that  $\psi$  is an atypical nonequilibrium state and that  $\psi(t)$  is a nonequilibrium processes of thermalization. So that such  $\psi(t)$  does exist,  $S(\psi)$  should at least satisfy the following condition:

(S3)  $dS(\psi(t))/dt|_{t=0} \neq 0$  for some  $\psi$  with finite probability for finite  $V$ .

Now we proceed to introduce the general formalism of the Boltzmann entropy  $S(\psi)$  for both classical and quantum systems. We start with the formalism for classical systems. Let  $\Gamma$  be the phase space of a classical systems. For every state  $\psi \in \Gamma$ , we assign a function  $f(\phi; \psi)$  of the state  $\phi \in \Gamma$ , which satisfies the properties of a probability density function with respect to  $\phi$ , i.e.,

$$\int_{\Gamma} d\phi f(\phi; \psi) = 1, \quad f(\phi; \psi) \geq 0. \quad (4)$$

We call the function  $f(\phi; \psi)$  the density function associated with the microscopic state  $\psi$ . This function  $f(\phi; \psi)$  should be distinguished from the PDF  $P^{(X)}(\phi)$  ( $\phi \in \Gamma$ ) associated with macroscopic thermodynamic state  $X$ . Hereinafter, we use the symbol “ $f$ ” for the density function associated with an individual microscopic state in order to avoid confusion. A Boltzmann entropy  $S(\psi)$ , i.e., entropy as a function of microscopic state, can be introduced as

$$S(\psi) = - \int_{\Gamma} d\phi f(\phi; \psi) \ln f(\phi; \psi). \quad (5)$$

The Boltzmann entropy  $S(\psi)$  is completely determined by the choice of the function  $f(\phi; \psi)$ . The function  $f(\phi; \psi)$  should be determined so as the corresponding Boltzmann entropy  $S(\psi)$  to satisfy the desirable conditions (S1)–(S3). A conceptual guideline to determine  $f(\phi; \psi)$  may be given by introducing a notion of “macroscopic similarity.” For a fixed state  $\psi$ , assign a value of  $f(\phi; \psi)$  for every state  $\phi$  according to the degree of macroscopic similarity between  $\phi$  and  $\psi$ . That is, let  $f(\phi; \psi) > f(\phi'; \psi)$  if  $\phi$  is macroscopically more similar to  $\psi$  in comparison with  $\phi'$ . Conversely, if  $f(\phi; \psi)$  is already defined, we may estimate the degree of the macroscopic similarity of  $\phi$  to  $\psi$  by the value of  $f(\phi; \psi)$ .

When a decomposition of the phase space  $\Gamma = \bigcup_v \Gamma_v$  into mutually disjoint subregions  $\Gamma_v$  is given and states in a same subregion may be regarded to be macroscopically similar to each other, one can define the function  $f(\phi; \psi)$  as

$$f(\phi; \psi) = |\Gamma_{v(\psi)}|^{-1} \delta_{v(\phi)v(\psi)}, \quad (6)$$

where  $|\Gamma_v|$  is the volume of  $\Gamma_v$ ,  $v(\psi)$  and  $v(\phi)$  are such that  $\psi \in \Gamma_{v(\psi)}$ , and  $\phi \in \Gamma_{v(\phi)}$ , respectively, and  $\delta_{vv'}$  is the Kronecker delta. Equation (5) reduces to

$$S(\psi) = \ln |\Gamma_{v(\psi)}|. \quad (7)$$

A decomposition of the phase space is obtained by specifying a sequence of the energy values  $U^{(v)}$  ( $v = 0, 1, 2, \dots$ ) satisfying  $U^{(0)} < U^{(1)} < U^{(2)} < \dots$  with  $U^{(0)}$  being the ground energy and letting  $\Gamma_v = \{\psi | U^{(v-1)} < H(\psi) \leq U^{(v)}\}$  ( $v = 1, 2, \dots$ ) where  $H(\psi)$  is the Hamiltonian. Then  $S(\psi)$  in

Eq. (7) is consistent with the Gibbs entropy for the micro-canonical ensemble  $S_{mc}(U)$  with  $U = H(\psi)$ . Another example of decomposition is given by introducing a set of real functions  $\{M\}(\psi) = \{M_1(\psi), \dots, M_n(\psi)\}$  which corresponds to macroscopic quantities. Let the sequences  $M_m^{(v_m)}$  ( $v_m = 0, 1, 2, \dots; m = 1, 2, \dots, n$ ) satisfy  $M_m^{(0)} < M_m^{(2)} < \dots$ , and the subregion is defined by  $\Gamma_v = \{\psi | M_m^{(v_m-1)} < M_m(\psi) \leq M_m^{(v_m)}, m = 1, \dots, n\}$  for  $v = \{v_1, \dots, v_m\}$ . Then  $S(\psi)$  in Eq. (7) is nothing but the Boltzmann entropy  $S_B(\{M\}(\psi))$  given in Ref. [11].

The equivalent formalism for quantum systems is given as follows: Let  $\mathcal{H}$  be the Hilbert space and we assign an operator  $f(\psi)$  to every pure state  $|\psi\rangle \in \mathcal{H}$  which satisfies the properties of density operator, i.e., self-adjoint, positive semidefinite, and of trace one. Again, we will use the symbol  $f$  for the density operator associated with individual pure state to distinguish it from the density operator  $\rho(X)$  associated with macroscopic thermodynamic state  $X$ . A Boltzmann entropy  $S(\psi)$  is given by

$$S(\psi) = -\text{tr}[f(\psi) \ln f(\psi)]. \quad (8)$$

The operator  $f(\psi)$  can be expressed as

$$f(\psi) = \int d\phi w(\phi; \psi) U(\phi; \psi) |\psi\rangle \langle \psi| U^\dagger(\phi; \psi), \quad (9)$$

where  $\phi$  is a parameter which may have many components,  $U(\phi; \psi)$  is a unitary operator labeled by  $\phi$  and  $\psi$ , and  $w(\phi; \psi) \geq 0$  is a weighting function satisfying  $\int d\phi w(\phi; \psi) = 1$ . The unitary operator  $U(\phi; \psi)$  maps the state  $|\psi\rangle$  to  $U(\phi; \psi)|\psi\rangle$  and the value of  $w(\phi; \psi)$  gives the degree of macroscopic similarity of  $U(\phi; \psi)|\psi\rangle$  to  $|\psi\rangle$ . The Boltzmann entropy is completely determined by  $U(\phi; \psi)$  and  $w(\phi; \psi)$  so that the problem is the choice of them.

For example, let us consider the case when a decomposition of the Hilbert space  $\mathcal{H}$  into mutually orthogonal  $n$  subspaces  $\mathcal{H}_v$  ( $v = 1, \dots, n$ ), i.e.,  $\mathcal{H} = \bigoplus_{v=1}^n \mathcal{H}_v$ , where  $n$  can be infinite, is given according to VN29. Let  $\mathcal{U}(\mathcal{H}_v)$  be the set of unitary operators acting on  $\mathcal{H}_v$  and  $\mu_v$  be the Haar measure on  $\mathcal{U}(\mathcal{H}_v)$  normalized as  $\int_{U_v \in \mathcal{U}(\mathcal{H}_v)} d\mu_v(U_v) 1 = 1$ . Let  $U_v \in \mathcal{U}(\mathcal{H}_v)$  and let the parameter  $\phi$  be  $\{U_v\} = \{U_1, U_2, \dots, U_n\}$ . We put  $U(\phi = \{U_v\}; \psi) = \prod_{v=1}^n U_v$  and  $d\phi w(\phi; \psi) = \prod_{v=1}^n d\mu_v(U_v)$ . Note that  $U(\phi; \psi)$  and  $w(\phi; \psi)$  are now independent of  $\psi$ . By noting that

$$\int_{\mathcal{U}(\mathcal{H}_v)} d\mu_v(U_v) U_v A U_v^\dagger = \frac{\text{tr}[P_v A P_v]}{\text{tr}[P_v]} P_v + (I - P_v) A (I - P_v), \quad (10)$$

where  $P_v$  is the projection operator on  $\mathcal{H}_v$ , and  $I$  is the identity operator on  $\mathcal{H}$ , one obtains

$$f(\psi) = \sum_v \frac{\text{tr}[P_v |\psi\rangle \langle \psi| P_v]}{\text{tr}[P_v]} P_v, \quad (11)$$

$$S(\psi) = - \sum_v \text{tr}[P_v |\psi\rangle \langle \psi| P_v] \ln \frac{\text{tr}[P_v |\psi\rangle \langle \psi| P_v]}{\text{tr}[P_v]}. \quad (12)$$

### III. NORMAL DISTRIBUTION MODEL FOR THE ENSEMBLE OF PURE STATES

As mentioned in Sec. II, we need an ensemble of pure states, or PDF  $P^{(X)}(\psi)$  on the Hilbert space  $\mathcal{H}$ , which corresponds to a given thermodynamic equilibrium state  $X$  in the case of quantum systems. The density operator  $\rho(X)$  that corresponds to a thermodynamic equilibrium state  $X$  can be obtained through the standard method of microcanonical ensemble, canonical ensemble, or some other variant ensembles. In this section, we introduce a method to construct the PDF  $P_N^{(X)}(\psi)$  from  $\rho(X)$ , where the subscript  $N$  stands for the normal distribution.

For a given density operator  $\rho$ , the way to decompose it into an ensemble, i.e., a weighted sum, of pure states  $\rho = \sum_{\alpha} P(\alpha)|\alpha\rangle\langle\alpha|$ , is not unique. The spectral decomposition is an evident example, but there are many other choices. Here, we introduce a decomposition which yields a multivariate complex normal distribution  $P_N(\psi)$  on the Hilbert space  $\mathcal{H}$ , i.e.,

$$\rho = \int_{\mathcal{H}} d\psi P_N(\psi)|\psi\rangle\langle\psi|, \quad (13)$$

$$P_N(\psi) = \frac{1}{\pi^D \det \rho} \exp[-\langle\psi|\rho^{-1}|\psi\rangle], \quad (14)$$

where  $d\psi = \prod_{\alpha=1}^D d\text{Re}\psi_{\alpha} d\text{Im}\psi_{\alpha}$ ,  $\psi_{\alpha} = \langle\alpha|\psi\rangle$ ,  $|\alpha\rangle$  ( $\alpha = 1, \dots, D$ ) is an arbitrary orthonormal basis,  $\det \rho$  is the determinant of a matrix expression of  $\rho$ , and  $D$  is the dimension of the Hilbert space  $\mathcal{H}$ . Equation (14) implies that the components  $\psi_{\alpha}$  obey the multivariate complex normal distribution with the means  $\overline{\psi_{\alpha}} = 0$  and the covariances  $\overline{\psi_{\alpha}\psi_{\beta}^*} = \langle\alpha|\rho|\beta\rangle$ . Then, it is easily checked that Eq. (13) holds by computing the matrix elements  $\langle\alpha|\bullet|\beta\rangle$  of the both sides. When  $\rho$  has 0 eigenvalue for an eigenvector  $|\alpha\rangle$ ,  $P(\psi)$  in Eq. (14) is not well defined. In such a case, we may put  $\rho|\alpha\rangle = \epsilon_{\alpha}|\alpha\rangle$  with  $\epsilon_{\alpha} > 0$  in Eq. (14) and the right-hand-side of Eq. (13) is safely obtained by taking the limit  $\epsilon_{\alpha} \rightarrow +0$ . For the case of  $D = \infty$ , we can first restrict the Hilbert space to be a finite-dimensional subspace  $\mathcal{H}' \subset \mathcal{H}$  and consider the projection of  $|\psi\rangle$  onto  $\mathcal{H}'$  and then increase the dimension of  $\mathcal{H}'$  to infinity. Equation (13) implies that  $\rho$  is equivalent to the ensemble of pure states  $|\psi\rangle$  with the probability density function (14).

Although we have  $\langle\psi|\psi\rangle = 1$ , individual states  $|\psi\rangle$  in the ensemble are not normalized:  $\langle\psi|\psi\rangle \neq 1$ , in general. However, if  $(\Delta\langle\psi|\psi\rangle)^2 := (\langle\psi|\psi\rangle - \overline{\langle\psi|\psi\rangle})^2$  is small enough, then  $|\psi\rangle$  is normalized as  $\langle\psi|\psi\rangle = 1$  with a sufficiently small deviation with probability almost 1. Let us consider the case for the canonical density operator  $\rho^{\text{can}}(\beta, V, N) := \exp[-\beta H(V, N)]/Z(\beta, V, N)$  where  $H(V, N)$  is the Hamiltonian and  $Z(\beta, V, N) := \text{tr}\{\exp[-\beta H(V, N)]\}$  is the partition function. It can be shown that  $(\Delta\langle\psi|\psi\rangle)^2 = Z(2\beta, V, N)/[Z(\beta, V, N)]^2 = \exp\{-2\beta[F(2\beta, V, N) - F(\beta, V, N)]\}$ , where  $F(\beta, V, N) = -\beta^{-1} \ln Z(\beta, V, N)$  is the Helmholtz free energy. For thermodynamically sound systems, we have  $F(\beta, V, N) = O(V)$  for  $V \rightarrow \infty$ ,  $\partial F(\beta, V, N)/\partial\beta = \beta^{-2}S(\beta, V, N)$ , and the entropy  $S(\beta, V, N)$  can be chosen to be positive for  $0 \leq \beta < \infty$ . Therefore, we have  $(\Delta\langle\psi|\psi\rangle)^2 \sim \exp[-f(\beta)V]$  with a function  $f(\beta)$  of  $\beta$  satisfying  $f(\beta) \geq 0$ , which

implies that  $\langle\psi|\psi\rangle = 1$  is satisfied with probability 1 in the thermodynamic limit  $V \rightarrow \infty$  for  $0 \leq \beta < \infty$ .

When  $\rho$  can be written in the form  $\rho = |J|^{-1} \sum_{j \in J} |j\rangle\langle j|$  where  $J$  is a set with the size  $|J| < \infty$  and  $\langle j|j'\rangle = \delta_{jj'}$ , there is another choice of PDF on the Hilbert space. The PDF is given by the uniform distribution on the surface of hypersphere  $\langle\psi|\psi\rangle = 1$  in the subspace  $\mathcal{H}_J$  which is spanned by  $|j\rangle$  ( $j \in J$ ). When all the thermodynamic variables in  $X$  are extensive variables such as the internal energy  $U$ , the microcanonical density operator  $\rho^{\text{mc}}(X)$  may be written in the above form with  $\mathcal{H}_J$  being the subspace spanned by the energy eigenvectors with the eigenvalues lying in  $((1 - \delta)U, U]$  where  $0 < \delta \ll 1$  and thermodynamic variables in  $X$  other than  $U$  (such as volume  $V$  or particle number  $N$ ) are fixed. We denote the PDF by  $P_{\text{sp}}^{(X)}(\psi)$  where the subscript ‘‘sp’’ stands for ‘‘hypersphere.’’ This type of PDF is often used in the context of typicality (see, e.g., Refs. [2–4]).

In the present study, we consider the case such that inverse temperature  $\beta$  rather than internal energy  $U$  is used to specify the thermodynamic state and the corresponding density operator is the canonical density operator, for which the model PDF that is uniformly distributed on a hypersphere cannot be applied straightforwardly (but, see Refs. [8,9] for some attempts to define an ensemble of pure states corresponding to canonical ensembles). Therefore, we use a normal distribution model PDF in the present study. Although it has the disadvantage that each pure state is not normalized in the strict sense, it has the advantage that some properties of normal distribution enable us to push forward the computation in Sec. V.

### IV. QUANTUM FIELD SYSTEMS

Let the spatial domain of the system be a  $d$ -dimensional cube with sides of length  $L$  applied with periodic boundary conditions. The volume of domain is  $V = L^d$ . Let the spatial coordinate be discretized with unit length  $\Delta x$  in each direction and let  $\mathcal{K}$  be the set of correspondingly discretized wave vectors,  $\mathbf{k} = (n_1, \dots, n_d)\Delta k$  where  $\Delta k = 2\pi/L$  and  $n_j = -L/2\Delta x, -L/2\Delta x + 1, \dots, L/2\Delta x - 1$  ( $j = 1, \dots, d$ ). The number of elements of  $\mathcal{K}$ , which is same as the number of lattice points in the spatial domain, is  $V(\Delta x)^{-d}$ . In the following, the thermodynamic limit will be taken by  $V \rightarrow \infty$  with fixed  $\Delta x$  or, equivalently,  $\Delta k \rightarrow 0$  with fixed  $k_{\text{max}} := \sqrt{d}\pi/\Delta x$ .

We consider a bosonic or fermionic field in this domain. Annihilation and creation operators,  $a_{\mathbf{k}}$  and  $a_{\mathbf{k}}^{\dagger}$ , respectively, associated with the wave vector  $\mathbf{k}$  satisfy the commutation relation  $[a_{\mathbf{k}}, a_{\mathbf{k}'}^{\dagger}] = \delta_{\mathbf{k},\mathbf{k}'}$  for bosonic fields, and the anticommutation relation  $\{a_{\mathbf{k}}, a_{\mathbf{k}'}^{\dagger}\} = \delta_{\mathbf{k},\mathbf{k}'}$  for fermionic fields, where  $\delta_{\mathbf{k},\mathbf{k}'}$  is the Kronecker delta in the vector space, i.e.,  $\delta_{\mathbf{k},\mathbf{k}'} = 1$  for  $\mathbf{k} = \mathbf{k}'$  and  $\delta_{\mathbf{k},\mathbf{k}'} = 0$  otherwise. Let  $\{n\}$  be a list of numbers  $n_{\mathbf{k}}$  ( $\mathbf{k} \in \mathcal{K}$ ) and  $|\{n\}\rangle$  be the Fock state,

$$|\{n\}\rangle := \prod_{\mathbf{k}} \frac{(a_{\mathbf{k}}^{\dagger})^{n_{\mathbf{k}}}}{\sqrt{n_{\mathbf{k}}!}} |0\rangle, \quad (15)$$

where  $|0\rangle$  is the vacuum specified by  $a_{\mathbf{k}}|0\rangle = 0$  ( $\mathbf{k} \in \mathcal{K}$ ),  $0 \leq n_{\mathbf{k}} < \infty$  for bosonic fields and  $n_{\mathbf{k}} = 0, 1$  for fermionic fields, and  $\prod'_{\mathbf{k}}$  denotes an ordered multiplication according to an arbitrary rule. Note that the rule is required to eliminate the

ambiguity of the sign for the case of fermionic fields. The Fock states  $|\{n\}\rangle$  with  $0 \leq \sum_k n_k < \infty$  form an orthonormal basis of the Hilbert space  $\mathcal{H}$  of the field system.

We assume that the Hamiltonian  $H$  of the field is invariant under the global phase translation  $a_k \rightarrow a_k e^{i\theta}$  for arbitrary  $\theta \in \mathbb{R}$  and the spatial translation  $a_k \rightarrow a_k e^{-ik \cdot \delta x}$  for arbitrary  $\delta x \in \mathbb{R}^d$ . These imply that the Hamiltonian  $H$  commutes with the particle number  $\hat{N} := \sum_k a_k^\dagger a_k$  and the momentum  $\mathbf{p} := \sum_k \mathbf{k} a_k^\dagger a_k$ . The explicit form of the Hamiltonian up to fourth order in the field operators is given by

$$H = \sum_k \omega_k a_k^\dagger a_k + \frac{1}{2} \sum_{kqrs} g_{kqrs} \delta_{k+q,r+s} a_k^\dagger a_q^\dagger a_r a_s, \quad (16)$$

where  $\omega_k \geq 0$  and  $g_{kqrs} \in \mathbb{C}$ . In general,  $H$  may contain higher-order terms in  $a_k$  and  $a_k^\dagger$ . We assume that  $\omega_k$  and  $g_{kqrs}$  and higher-order coefficients are prescribed in the domain of continuous-wave vector space and that they are continuous functions of the wave vectors. Let  $|j\rangle$  ( $j = 0, 1, 2, \dots$ ) be simultaneous eigenstates of the particle numbers  $\hat{N}$ , momentum  $\mathbf{p}$ , and the Hamiltonian  $H$  with the eigenvalues  $N_j$ ,  $\mathbf{p}_j$ , and  $E_j$ , respectively. When some of the energy eigenstates are degenerate, i.e.,  $N_j = N_{j'}$ ,  $\mathbf{p}_j = \mathbf{p}_{j'}$ , and  $E_j = E_{j'}$  for  $j \neq j'$ , we choose  $|j\rangle$  and  $|j'\rangle$  to be orthogonal so that all  $|j\rangle$ s form an orthonormal basis of the Hilbert space  $\mathcal{H}$  of the field system. The Fock states  $|\{n\}\rangle$  may be used as an orthonormal basis  $|j\rangle$  for free-field systems, i.e.,  $H = \sum_k \omega_k a_k^\dagger a_k$ , but the orthonormal basis  $|j\rangle$  does not coincide with the Fock states  $|\{n\}\rangle$  for general (self-)interacting field systems.

Hereafter, we consider the thermodynamic state  $(\beta, V, N)$ . Let  $\mathcal{H}_N$  be the subspace of  $\mathcal{H}$  spanned by the eigenstates of  $\hat{N}$  with the eigenvalue  $N$ . We restrict the Hilbert space to  $\mathcal{H}_N$  for the thermodynamic equilibrium state  $(\beta, V, N)$  and the thermodynamic limit  $V \rightarrow \infty$  will be taken with fixed  $N/V$ .

## V. BOLTZMANN ENTROPY FOR QUANTUM FIELD SYSTEMS

Let the unitary operator  $U_\Theta$  parametrized by  $\Theta = (\theta_0, \theta_1, \theta_2, \dots)$  ( $0 \leq \theta_j < 2\pi$ ) be given by

$$U_\Theta |j\rangle = \sum_j e^{i\theta_j} |j\rangle. \quad (17)$$

Let  $U_\kappa$  be the unitary operator which shifts the field in the wave-vector space by a wave vector  $\kappa \in \mathcal{K}'$ , i.e.,

$$U_\kappa a_k U_\kappa^\dagger = a_{k+\kappa}, \quad (18)$$

where  $\mathcal{K}'$  is a set of wave vectors  $\kappa$  satisfying  $\kappa = (n_1, \dots, n_d) \Delta k$  with  $n_j = -[\zeta L/2\Delta x]$ ,  $-[\zeta L/2\Delta x] + 1, \dots, [\zeta L/2\Delta x]$ , and  $\zeta$  is a positive small parameter. Hereafter, we identify the wave vector  $\mathbf{k} + (2\pi/\Delta x)\boldsymbol{\ell}$  ( $\boldsymbol{\ell} \in \mathbb{Z}^d$ ) with  $\mathbf{k}$  so that all wave vectors under consideration belong to  $\mathcal{K}$ . Note that  $U_\kappa^\dagger = U_{-\kappa}$ . Provided that the vacuum  $|0\rangle$  is invariant under the operation of  $U_\kappa$  for  $\kappa \in \mathcal{K}'$ , the operator  $U_\kappa$  transfers a Fock state  $|\{n\}\rangle$  to another Fock state  $U_\kappa |\{n\}\rangle = \prod_k (a_{k+\kappa}^\dagger)^{n_k} / \sqrt{n_k!} |0\rangle$ . In the thermodynamic limit, we put  $\zeta = \zeta_0 (L/\Delta x)^{-\alpha} = \zeta_0 V^{-\alpha/d} (\Delta x)^\alpha$  with  $0 < \alpha < 1$  and a positive small constant  $\zeta_0$ . Note that  $\kappa_{\max} := \sqrt{d} [\zeta L/2\Delta x] \Delta k$  scales as  $\kappa_{\max} = O(V^{-\alpha/d})$  and the size of the set  $\mathcal{K}'$  scales as  $|\mathcal{K}'| \propto V^{1-\alpha}$ .

Let the operator  $f(\psi)$  associated with a state  $|\psi\rangle$  be given by

$$\begin{aligned} f(\psi) &= \left( \prod_j \int_0^{2\pi} \frac{d\theta_j}{2\pi} \right) \frac{1}{|\mathcal{K}'|} \sum_\kappa U_\Theta U_\kappa |\psi\rangle \langle \psi | U_\kappa^\dagger U_\Theta^\dagger \\ &= \frac{1}{|\mathcal{K}'|} \sum_j \sum_\kappa \mathbf{P}_j U_\kappa |\psi\rangle \langle \psi | U_\kappa^\dagger \mathbf{P}_j, \end{aligned} \quad (19)$$

where  $\mathbf{P}_j := |j\rangle \langle j|$  is the projection operator and we used Eq. (10) in the second equality. We propose to define the Boltzmann entropy  $S(\psi)$  for quantum field systems as Eq. (8) with Eq. (19). We will see that, under an assumption specified later, the proposed Boltzmann entropy  $S(\psi)$  satisfies the properties (S1)–(S3) with respect to the ensemble of pure states given by the PDF  $P_N^{(\beta, V, N)}(\psi)$ , that is, the normal distribution model for the canonical density operator  $\rho^{\text{can}}(\beta, V, N)$  associated with the thermodynamic state  $(\beta, V, N)$ . In the rest of this section,  $(\beta, V, N)$  is denoted by  $\gamma$  for convenience.

From Eq. (19), we have

$$\langle j | f(\psi) | j' \rangle = f_j(\psi) \delta_{jj'}, \quad (20)$$

$$f_j(\psi) = \frac{1}{|\mathcal{K}'|} \sum_{\kappa \in \mathcal{K}'} | \langle j | U_\kappa | \psi \rangle |^2. \quad (21)$$

Let  $H_\kappa := U_\kappa H U_\kappa^\dagger$  and  $\delta_\kappa H := H_\kappa - H$ . The general expression of  $H_\kappa$  up to fourth order in the field operators is given by

$$H_\kappa = \sum_k \omega_{k-\kappa} a_k^\dagger a_k + \frac{1}{2} \sum_{kpqr} g_{k-\kappa, p-\kappa, q-\kappa, r-\kappa} \delta_{k+p, q+r} a_k^\dagger a_p^\dagger a_q a_r. \quad (22)$$

Let  $\rho_\kappa^{\text{can}}(\gamma) := U_\kappa \rho^{\text{can}}(\gamma) U_\kappa^\dagger = \exp[-\beta(H + \delta_\kappa H)]/Z(\gamma)$  and define an operator  $A_\kappa(\gamma)$  by

$$\rho_\kappa^{\text{can}}(\gamma) = \rho^{\text{can}}(\gamma) [I + \lambda A_\kappa(\gamma)], \quad (23)$$

where  $I$  is the identity operator and  $\lambda = 1$  is a bookkeeping parameter. Since  $\omega_k$ ,  $g_{kqrs}$ , and the higher-order coefficients in  $H$  are continuous in the wave vectors  $\mathbf{k}$ , we have  $A_\kappa(\gamma) = O(\kappa)$  for  $\kappa \rightarrow 0$  where  $\kappa := |\kappa|$ .

Since we use the normal distribution model  $P_N^{(\gamma)}(\psi)$ , the coefficients  $\psi_j = \langle j | \psi \rangle$  obey the multivariate complex normal distribution with the means  $\overline{\psi_j^{(\gamma)}} = 0$  and the covariances  $\overline{\psi_j \psi_{j'}^*}^{(\gamma)} = \rho_j^{\text{can}}(\gamma) \delta_{jj'}$  where  $\rho_j^{\text{can}}(\gamma) := \langle j | \rho^{\text{can}}(\gamma) | j \rangle = \exp[-\beta E_j]/Z(\gamma)$ . From Eqs. (21) and (23), we have

$$\overline{f_j(\psi)}^{(\gamma)} = \rho_j^{\text{can}}(\gamma) \left( 1 + \frac{\lambda}{|\mathcal{K}'|} \sum_{\kappa \in \mathcal{K}'} \langle j | A_\kappa(\gamma) | j \rangle \right). \quad (24)$$

Let  $\Delta f_j(\psi) := f_j(\psi) - \overline{f_j(\psi)}^{(\gamma)}$  be the fluctuation and  $C_{j_1 j_2 \dots j_m}(\gamma) := \overline{\Delta f_{j_1}(\psi) \Delta f_{j_2}(\psi) \dots \Delta f_{j_m}(\psi)}^{(\gamma)}$  be the associated  $m$ th order moments. In virtue of the multivariate complex normal distribution of  $\psi_j$ ,  $C_{j_1 j_2 \dots j_m}(\gamma)$  can be

expressed as

$$C_{j_1 j_2 \dots j_m}(\gamma) = \frac{1}{|\mathcal{K}'|^m} \sum_{\sigma \in \mathcal{P}} \left( \prod_{m'=1}^m \sum_{\kappa_{m'} \in \mathcal{K}'} \right) \times \left( \prod_{m'=1}^m \langle j_{m'} | \rho_{\kappa_{m'}}^{\text{can}}(\gamma) U_{\kappa_{m'} - \kappa_{\sigma(m')}} | j_{\sigma(m')} \rangle \right), \quad (25)$$

where  $\mathcal{P}$  is the set of permutations of  $\{1, 2, \dots, m\}$  without fixed points. Note that  $\langle j | \rho_{\kappa}^{\text{can}}(\gamma) U_{\kappa - \kappa'} | j' \rangle \neq 0$  only if  $\mathbf{p}_j - N\boldsymbol{\kappa} = \mathbf{p}_{j'} - N\boldsymbol{\kappa}'$ . For fixed  $j, j'$ , and  $\boldsymbol{\kappa}$  there is at most one  $\boldsymbol{\kappa}'$  that satisfies the above condition. There are  $|\mathcal{K}'|^m = O(V^{m(1-\alpha)})$  terms in the summation  $\prod_{m'=1}^m \sum_{\kappa_{m'} \in \mathcal{K}'}$ , but at most  $O(|\mathcal{K}'|^{m/2}) = O(V^{m(1-\alpha)/2})$  terms are not 0. The fact is essential in the following estimates.

The Boltzmann entropy  $S(\psi)$  depends on  $\psi$  only through  $f(\psi)$  as  $S(\psi) = \sum_j S_1(f_j(\psi))$  where  $S_1(x) := -x \ln x$ . Let us introduce bounding functions  $S_1^{(u)}(x, y) := -y \ln y - (1 + \ln y)(x - y)$  and  $S_1^{(\ell)}(x, y) := S_1^{(u)}(x, y) - y^{-1}(x - y)^2$ , which are polynomial in  $x$  and satisfy  $S_1^{(\ell)}(x, y) \leq S_1(x) \leq S_1^{(u)}(x, y)$  for  $x, y > 0$ . By substituting  $x = f_j(\psi)$  and  $y = \overline{f_j(\psi)}^{(\gamma)}$  into the inequalities, taking the average with respect to the

thermodynamic state  $\gamma$  and summing over  $j$  yields

$$\begin{aligned} \sum_j [S_1(\overline{f_j(\psi)}^{(\gamma)}) - (\overline{f_j(\psi)}^{(\gamma)})^{-1} C_{jj}(\gamma)] &\leq \overline{S(\psi)}^{(\gamma)} \\ &\leq \sum_j S_1(\overline{f_j(\psi)}^{(\gamma)}). \end{aligned} \quad (26)$$

The upper and lower bounds in the inequalities (26) can be expanded in a power series of  $\lambda$  by using Eqs. (23)–(25). Each  $O(\lambda)$  term contains  $A_{\boldsymbol{\kappa}}(\gamma)$  whose components  $\langle j | A_{\boldsymbol{\kappa}}(\gamma) | j' \rangle$  are  $O(\kappa)$  for fixed  $V$ . Here we employ the following assumption:

(A1)  $O(\lambda)$  terms appearing in the estimate of  $\overline{S(\psi)}^{(\gamma)}$  and  $[\Delta S(\psi)]^2^{(\gamma)}$  can be neglected in the thermodynamic limit  $V \rightarrow \infty$  with  $\kappa_{\text{max}} = O(V^{-\alpha/d})$ .

Under assumption (A1),  $\overline{f_j(\psi)}^{(\gamma)}$  and  $C_{jj}(\gamma)$  in Eq. (26) can be replaced by  $\rho_j^{\text{can}}(\gamma)$  and  $|\mathcal{K}'|^{-1} [\rho_j^{\text{can}}(\gamma)]^2$ , respectively. Thus, we arrive at

$$\overline{S(\psi)}^{(\gamma)} = S(\gamma) + O(V^{-(1-\alpha)}), \quad (27)$$

which implies that (S1) is satisfied.

For the estimate of  $[\Delta S(\psi)]^2^{(\gamma)}$ , we introduce a function  $\Delta S_1(x, y) := S_1(x) - S_1(y)$  and a bounding function  $\Delta S_1^{2(u)}(x, y) := [(1 - 2 \ln y)/2y]^2 (x^2 - y^2)^2$  such that  $[\Delta S_1(x, y)]^2 \leq \Delta S_1^{2(u)}(x, y)$  for  $x, y > 0$ . We have

$$\begin{aligned} \overline{[\Delta S(\psi)]^2}^{(\gamma)} &= \sum_{jj'} \overline{\Delta S_1(f_j(\psi), \overline{f_j(\psi)}^{(\gamma)}) \Delta S_1(f_{j'}(\psi), \overline{f_{j'}(\psi)}^{(\gamma)})}^{(\gamma)} - \left[ \sum_j \overline{\Delta S_1(f_j(\psi), \overline{f_j(\psi)}^{(\gamma)})}^{(\gamma)} \right]^2 \\ &\leq \left\{ \sum_j \overline{[\Delta S_1^{2(u)}(f_j(\psi), \overline{f_j(\psi)}^{(\gamma)})]^{1/2}}^{(\gamma)} \right\}^2, \end{aligned} \quad (28)$$

where we used the Cauchy-Schwarz inequality and the bounding inequality regarding  $\Delta S_1^{2(u)}(x, y)$  in the last inequality. The right-hand side of inequality (28) can be written in terms of the moments  $C_{j_1 j_2 \dots j_m}(\gamma)$  in Eq. (25). By applying assumption (A1) to inequality (28), we can show that

$$\frac{\overline{[\Delta S(\psi)]^2}^{(\gamma)}}{S(\gamma)^2} = O(V^{-(1-\alpha)}), \quad (29)$$

which implies that (S2) is satisfied.

Regarding the dynamics, we have

$$f_j(\psi(t)) = \frac{1}{|\mathcal{K}'|} \sum_{\boldsymbol{\kappa} \in \mathcal{K}'} \left| \sum_{j'} \langle j | U_{\boldsymbol{\kappa}} | j' \rangle \psi_{j'}(0) e^{-iE_j t} \right|^2. \quad (30)$$

In the case of free field systems,  $|j\rangle$  and  $|j'\rangle$  are Fock states and  $U_{\boldsymbol{\kappa}}^\dagger |j\rangle = U_{-\boldsymbol{\kappa}} |j\rangle$  is also a Fock state. Since the Fock states form an orthonormal basis,  $\langle j | U_{\boldsymbol{\kappa}} | j' \rangle \neq 0$  is satisfied for at most one  $j'$  for arbitrary fixed  $j$  and  $\boldsymbol{\kappa}$ . This implies that  $f_j(\psi(t))$  is independent of  $t$  for free field systems. For general (self-)interacting field systems, we have  $[H, H_{-\boldsymbol{\kappa}}] \neq 0$  for  $\boldsymbol{\kappa} \neq \mathbf{0}$ . Note that  $U_{-\boldsymbol{\kappa}} |j\rangle (j = 1, 2, \dots)$  are eigenstates of  $H_{-\boldsymbol{\kappa}}$ , and that there are some  $j$  such that  $\langle j | U_{\boldsymbol{\kappa}} | j' \rangle \neq 0$  for two

or more  $j'$ s. The element  $f_j(\psi)$  depends on  $t$  when  $\psi_{j'}(0) \neq 0$  for those  $j'$ s. Furthermore, the  $t$  dependence of  $f_j(\psi(t))$  leads to the  $t$  dependence of  $S(\psi(t))$ . Thus, (S3) is satisfied for (self-)interacting field systems.

## VI. DISCUSSIONS

A different and simpler definition of the Boltzmann entropy can be given by substituting

$$\begin{aligned} f_d(\psi) &= \left( \prod_{j=1}^D \int_0^{2\pi} \frac{d\theta_j}{2\pi} \right) U_{\Theta} |\psi\rangle \langle \psi | U_{\Theta}^\dagger, \\ &= \sum_j P_j |\psi\rangle \langle \psi | P_j, \end{aligned} \quad (31)$$

into  $f(\psi)$  of Eq. (8). This type of entropy, denoted  $S_d(\psi)$ , is often called the diagonal entropy (see, e.g., Ref. [17]). It can be shown that  $S_d(\psi)$  satisfies (S1) and (S2) but fails to satisfy (S3), i.e.,  $S_d(\psi(t))$  do not depend on  $t$  under the Hamiltonian dynamics. In order that  $f(\psi(t))$  and  $S(\psi(t))$  depend on time, a parametrized set of unitary operators which do not commute with the Hamiltonian  $H$  is necessary. The situation is conceptually akin to selecting a decomposition

of the Hilbert space  $\mathcal{H}$  whose projection operators  $P_\nu$  do not commute with  $H$  in VN29. Furthermore, the introduction of the set of unitary operators should not violate (S1) and (S2). Following the preceding study on the Boltzmann entropy for classical field systems [14], we introduced the set of operators  $U_\kappa (\kappa \in \mathcal{K}')$  that shifts the field in the wave-vector space to fulfill the above requirements. The underlying idea of the operator  $U_\kappa$  may be given as follows: When the Hamiltonian  $H$  is invariant under the spatial translation and global phase translation, the correlation in the wave-vector space takes the form  $\text{tr}[a_k^\dagger a_{k'} \rho^{\text{can}}(\beta, V, N)] = G_k \delta_{k,k'}$ ,  $\text{tr}[a_k a_{k'}^\dagger \rho^{\text{can}}(\beta, V, N)] = \text{tr}[a_k^\dagger a_{k'}^\dagger \rho^{\text{can}}(\beta, V, N)] = 0$ . This implies that the different wave-vector modes are uncorrelated at the level of the second-order moments. When  $G_k$  is a smooth function of  $\mathbf{k}$ , which may be expected when  $\omega_k$  and higher-order coefficients in the Hamiltonian  $H$  are smooth, the neighboring wave-vector modes  $\mathbf{k}$  and  $\mathbf{k} + \kappa$  ( $\kappa \in \mathcal{K}'$ ) may be interpreted as statistically quasi-independent replicas of each other. The interacting wave-vector modes  $a_{k_1}, \dots, a_{k_m}, a_{k'_1}^\dagger, \dots, a_{k'_m}^\dagger$  satisfy the momentum-preserving condition  $\sum_{m'=1}^m \mathbf{k}_{m'} - \sum_{m'=1}^m \mathbf{k}'_{m'} = \mathbf{0}$  and the condition is not violated by a shift in the wave-vector space,  $\mathbf{k} \rightarrow \mathbf{k} + \kappa$ . Based on these considerations, it may be appropriate to regard that the states  $|\psi\rangle$  and  $U_\kappa |\psi\rangle$  ( $\kappa \in \mathcal{K}'$ ) “resemble” each other.

In the present study, we chose the set of thermodynamic variables  $(\beta, V, N)$  to specify a thermodynamic state and the corresponding canonical density operator  $\rho^{\text{can}}(\beta, V, N)$  is interpreted as an ensemble of unnormalized pure states  $P_N^{(\beta, V, N)}(\psi)$  using the normal distribution model. Exploiting this setting of the ensemble of pure states, we showed, with an additional assumption (A1), that (S1)–(S3) hold. When the set of thermodynamic variables  $(U, V, N)$ , where  $U$  is the internal energy, is chosen, the density operator may be given by that of the microcanonical ensemble  $\rho^{\text{mc}}(U, V, N) = |J_U|^{-1} \sum_{j \in J_U} |j\rangle \langle j|$ , where  $J_U$  is the set of indices  $j$  satisfying  $(1 - \delta)U < E_j \leq U$  with  $H|j\rangle = E_j|j\rangle$  and  $0 < \delta \ll 1$ , and  $|J_U|$  is the size of the set  $J_U$ . As mentioned in Sec. III, the model PDF  $P_{\text{sp}}^{(U, V, N)}$  which is distributed uniformly on the surface of a hypersphere may be used in this case. The PDF  $P_N^{(\beta, V, N)}(\psi)$  approximates  $P_{\text{sp}}^{(U(\beta, V, N), V, N)}(\psi)$  in the sense that  $(\Delta \langle \psi | \psi \rangle) \rightarrow 0$  for  $V \rightarrow \infty$  and that  $\Delta U(\beta, V, N)/U(\beta, V, N) = O(V^{-1/2})$ , where  $\Delta U(\beta, V, N) := (\text{tr}[\rho^{\text{can}}(\beta, V, N)[H - U(\beta, V, N)]^2])^{1/2}$ , holds for thermodynamically sound systems. Taking into account the resemblance of the two PDFs  $P_N^{(\beta, V, N)}(\psi)$  and  $P_{\text{sp}}^{(U(\beta, V, N), V, N)}(\psi)$ , it is probable that the properties (S1)–(S3) hold not only for  $P_N^{(\beta, V, N)}(\psi)$  but also for  $P_{\text{sp}}^{(U, V, N)}(\psi)$ . If (S1)–(S3) hold for  $P_{\text{sp}}^{(U, V, N)}(\psi)$ ,  $\Delta S(\psi) := S(\psi) - S(U = \langle \psi | H | \psi \rangle, V, N)$  would be almost 0 for almost all states  $|\psi\rangle$  with respect to the PDF  $P_{\text{sp}}^{(U, V, N)}(\psi)$ . We interpret these states as thermodynamic equilibrium states. Then,  $\Delta S(\psi)$  gives a measure of departure from the thermodynamic equilibrium. States with large  $|\Delta S(\psi)|$  correspond to nonequilibrium states. We hope that  $\Delta S(\psi) < 0$  for most nonequilibrium states and that the thermalization process corresponds to  $\lim_{t \rightarrow \infty} \Delta S(\psi(t)) = 0$  with  $dS(\psi(t))/dt > 0$ .

The eigenstate thermalization hypothesis (ETH) [18,19] states that a single energy eigenstate can behave as a thermal

state. In the present context, the ETH is given as  $\Delta S(\psi) \approx 0$  for almost all energy eigenstates  $|\psi\rangle = |j\rangle$ . One can see from Eqs. (8) and (19)–(21) that the expression of the operators  $U_\kappa$  ( $\kappa \in \mathcal{K}'$ ) in the energy eigenstate basis  $|j\rangle$ , that is  $\langle j' | U_\kappa | j \rangle$ , is required to compute  $S(j) := S(\psi)|_{|\psi\rangle=|j\rangle}$ . In the case of a free field system, there is only one  $j'$  such that  $\langle j' | U_\kappa | j \rangle \neq 0$  for every fixed  $j$  and we have  $S(j) = -\ln |\mathcal{K}'| \propto -(1 - \alpha) \ln V = o(V)$  and  $S(j) \neq S(U = E_j, V, N) = O(V)$ , which implies that the ETH is not valid for free fields. For general fields with interactions, there can be more than one  $j'$  such that  $\langle j' | U_\kappa | j \rangle \neq 0$  for every fixed  $j$ . If there are sufficiently many such  $j'$ 's, then there is a possibility that the ETH is valid for some fields with interactions. When the ETH is valid, nonequilibrium states  $|\psi\rangle$ , if they exist, are linear superpositions of energy eigenstates that are thermodynamic equilibrium states. Let us fix an initial state as  $|\psi(0)\rangle = \sum_j \psi_j(0) |j\rangle$ . Only when  $\psi_j(0)$  for various  $j'$  are in some special coherent relations between each other,  $f_j(\psi(t))$  in Eq. (30) with  $t = 0$  would take an atypical value. And when  $f_j(\psi(0))$  takes an atypical value for sufficiently many  $j$ 's,  $\Delta S(\psi(0))$  would deviate significantly from 0, i.e.,  $|\psi(0)\rangle$  is a nonequilibrium state. Even when  $|\psi(0)\rangle$  is a nonequilibrium state, the factors  $e^{-iE_j t}$  in Eq. (30) destroy the coherence for  $t > \epsilon$  with some small  $\epsilon (> 0)$  and  $\Delta S(\psi(t)) \approx 0$  would be achieved, which implies the thermalization. The present dynamical description of thermalization is consistent with that depicted in Fig. 2 of Ref. [7].

In ŠDA19, a coarse-graining in position space is introduced to construct a Boltzmann entropy for systems of many quantum particles. Let the spatial domain of the system  $\mathcal{D}$  be divided into disjoint subdomains  $\mathcal{D}_\ell$  ( $\ell = 1, 2, \dots$ ) corresponding to the coarse-graining. Let  $\hat{n}_\ell$  be the number operator of the particles in the subdomain  $\mathcal{D}_\ell$  and  $\mathcal{H}_\nu$  be the subspace of the Hilbert space  $\mathcal{H}$  that is spanned by the simultaneous eigenstates of  $\{\hat{n}_1, \hat{n}_2, \dots\}$  with the eigenvalues  $\nu = \{n_1, n_2, \dots\}$ . Let  $\mathbf{Q}_\nu$  be the projection operator on  $\mathcal{H}_\nu$  and  $\mathbf{P}_j = |j\rangle \langle j|$  where  $|j\rangle$  ( $j = 0, 1, 2, \dots$ ) are energy eigenstates. The observational entropy  $S_{x_E}(\psi)$  with coarse-graining in position space and fine-graining in energy in the terminology of ŠDA19 is formulated by

$$S_{x_E}(\psi) = - \sum_{\nu, j} \text{tr}[\mathbf{P}_j \mathbf{Q}_\nu |\psi\rangle \langle \psi| \mathbf{Q}_\nu \mathbf{P}_j] \times \ln \frac{\text{tr}[\mathbf{P}_j \mathbf{Q}_\nu |\psi\rangle \langle \psi| \mathbf{Q}_\nu \mathbf{P}_j]}{\text{tr}[\mathbf{P}_j \mathbf{Q}_\nu \mathbf{P}_j]}, \quad (32)$$

in analogy with Eq. (12). Note that  $S_{x_E}$  in ŠDA19 is defined for the general density matrix  $\rho$  but here we restrict it to be a function of a pure state  $\rho = |\psi\rangle \langle \psi|$ . Since  $\mathbf{P}_j$  and  $\mathbf{Q}_\nu$  do not commute in general, the density operator  $f_{x_E}(\psi)$  associated with the pure state  $\psi$  which satisfies  $S_{x_E}(\psi) = -\text{tr}[f_{x_E}(\psi) \ln f_{x_E}(\psi)]$  cannot be formulated in general. Thus,  $S_{x_E}(\psi)$  does not fit into the formalism given in Sec. II in a strict sense. However, we may discuss conceptual similarity and difference between the Boltzmann entropy  $S(\psi)$ , Eq. (8) with Eq. (19), proposed in the present paper and  $S_{x_E}(\psi)$  in ŠDA19. They are similar in the sense that they both use  $U_\Theta$ ,  $\mathbf{P}_j$ , or the fine-graining in energy in the terminology of ŠDA19. The difference between the two Boltzmann

entropies is that the shift in wave-vector space is used in  $S(\psi)$  while the coarse-graining in position space is used in  $S_{xE}(\psi)$ . The coarse-graining method is supposed to work well when the interaction between the particles is collisional or short ranged, so that  $S_{xE}(\psi)$  would not be appropriate when the interaction is long-ranged beyond the coarse-graining scale. The Boltzmann entropy  $S(\psi)$  in the present study has no limitation in the interacting scale range. On the other hand, the method of shift in the wave-vector space requires the invariance of the Hamiltonian under the spatial translation, so that  $S_{xE}(\psi)$  may be more suitable in the cases such that an external potential field depending on position is present. Many other definitions of Boltzmann entropy satisfying (S1)–(S3) would be possible. Actually, the examples of Boltzmann entropy other than  $S_{xE}(\psi)$  are given in ŠDA19. Among many

definitions, an appropriate one should be used depending on the situation.

The main purpose of this paper is to propose the Boltzmann entropy  $S(\psi)$  for quantum field systems given by Eq. (8) with Eq. (19) and to show its potential for characterizing nonequilibrium dynamical processes, including thermalization. Validation of the assumption (A1) and detailed analysis of  $\langle j'|U_k|j \rangle$  and ETH for some specific field systems are beyond the scope of the present study. They may be left for future studies.

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