Typicality and Statewise Entropy for Classical Field Systems

Kyo Yoshida
Institute of Physics, University of Tsukuba,
1-1-1 Tennoudai, Tsukuba, Ibaraki 305-8571, Japan

Reprint of *EPL* **110**(2015) 60001

Abstract

We consider a classical field system with discretized spatial coordinates and a quadratic Hamiltonian. Typicality for the system is shown in the sense that, for functions of state which satisfy certain conditions including the invariance under the spatial translations of the state, the values of the functions at almost all individual states in a microcanonical ensemble are almost equal to their microcanonical ensemble averages. A statewise entropy for the system is constructed in such a way that it satisfies the above conditions and its microcanonical average coincide with the entropy in standard formalism of statistical mechanics.

1 Typicality for classical field systems

In standard formalism of statistical mechanics, a thermal equilibrium state is described by an ensemble of states in the classical or quantum mechanical system. Recently, the justification of the ensemble description has been discussed by employing the concept of typicality. In general, typicality may be stated as follows. Consider an ensemble of states and functions of state such that their values at almost all individual states, called typical states, hardly deviate from their ensemble averages, then, as far as these functions are concerned, every typical state in the ensemble can represent the ensemble and inversely, the ensemble average can be utilized to obtain information of the typical states.

It is shown in Refs. [1, 2, 3, 4] that, for almost all pure states in the microcanonical ensemble of a large quantum system, the reduced density matrix of a small subsystem is very close to its microcanonical ensemble average, that is, the canonical density matrix.

In Ref. [5], the typicality is considered from a classical perspective. In its construction, the state space is discrete and an ensemble of probability distributions on the discrete state space is introduced. Then, the typicality with respect to this ensemble of probability distribution can be analyzed in a similar way as that of the quantum systems. However, in order to discuss the justification of the standard formalism of statistical mechanics, one must deal with the typicality with respect to the ensemble of states, such as the microcanonical ensemble. The relation between the typicality with respect to the ensemble of the probability distributions in Ref. [5] and that with respect to the ensemble of states in classical systems is not evident.

In this letter, we consider the typicality with respect to the microcanonical ensemble, an ensemble of states, for classical systems. We work in a field-theoretical formalism, that is, the degrees of freedom are labeled by spatial position. Let the spatial size of the system be finite and the spatial coordinates are discretized so that the total number of the degrees of freedom is finite. Since we consider real-valued fields, the state space, namely the phase space, is continuous in contrast to that considered in Ref. [5]. In all previous studies Refs. [1, 2, 3, 4, 5], they separate the total system into a subsystem and the bath, and the typicality is analyzed with respect to the functions of variables in the subsystem. In addition to that, functions of lower order moments of variables in the full system are considered in Refs. [1, 2]. In the present field-theoretical formalism, we take a different approach. The typicality is analyzed with respect to the functions of the state, namely the functionals of the field, that are invariant under spatial translations of the field.

The precise setting is given as follows. We consider a classical Hamiltonian system with real canonical coordinates $\hat{q}_\ell(\boldsymbol{x})$ and $\hat{p}_\ell(\boldsymbol{x})$ that are labeled by position $\boldsymbol{x}$ in a spatial domain and the index $\ell = 1, \cdots, M/2$ representing the other arbitrary degrees of freedom. We employ the notation $\hat{q}_{\ell+M/2}(\boldsymbol{x}) = \hat{p}_\ell(\boldsymbol{x})$ for convenience. The spatial domain is a d-dimensional cube with sides of length L applied with periodic boundary conditions. The spatial coordinate is discretized with the unit length Δx in each direction as $\boldsymbol{x} = (n_1\Delta x, \cdots, n_d\Delta x)(n_i = 0, \cdots, N-1)$ where $N = L/\Delta x$ is an integer. The total number of the degrees of freedom of this system is $\nu = MN^d$ where we counted $\hat{q}_\ell(\boldsymbol{x})$ and $\hat{q}_{\ell+M/2}(\boldsymbol{x}) = \hat{p}_\ell(\boldsymbol{x})$ as different degrees of freedom. The Fourier transform of $\hat{q}_\ell(\boldsymbol{x})$ is introduced by

$$q_\ell(\boldsymbol{k}) = \sum_{\boldsymbol{x}} (\Delta x)^d \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} \hat{q}_\ell(\boldsymbol{x}), \tag{1}$$

where $\boldsymbol{k} = (n_1\Delta k, \cdots, n_d\Delta k), n_i = (-N/2, -N/2+1, \cdots, 0, \cdots, N/2-1)$ and $\Delta k = 2\pi/L = 2\pi/N\Delta x$. We have $q_\ell(-\boldsymbol{k}) = q_\ell^*(\boldsymbol{k})$ from the reality of $\hat{q}_\ell(\boldsymbol{x})$. A state is specified by $\nu/2$ complex values $\{q\} = \{q_\ell(\boldsymbol{k})\}(\ell = 1, \cdots, M, \boldsymbol{k} \in \mathcal{K})$ where $\mathcal{K}$ is a set of $N^d/2$ wavevectors such that only either of $\boldsymbol{k}$ and $-\boldsymbol{k}$ is contained in it for each $\boldsymbol{k}(\neq \boldsymbol{0})$. In this letter, we take as $\mathcal{K} = \{\boldsymbol{k}|(n_1 > 0) \vee (n_1 = 0 \wedge n_2 > 0) \vee \cdots \vee (n_1 = \cdots = n_{d-1} = 0 \wedge n_d > 0) \vee (n_1 = \cdots = n_d = 0)\}$. Here, some wavevectors with $n_i = -N/2$ are neglected, but the number of those wavevectors are $O(N^{d-1})$ and its ratio to the total number of wavevectors vanishes as $N \to \infty$. Here and hereafter, the parameters d, M and Δx are fixed, and the system size is changed by changing N, or equivalently, L, ν or Δk.

We restrict the form of the Hamiltonian to be that of harmonic oscillators, i.e.

$$H(\{q\}) = 2\sum_{\boldsymbol{k}\in\mathcal{K},\ell} \left(\frac{\Delta k}{2\pi}\right)^d h_\ell(\boldsymbol{k}) q_\ell(\boldsymbol{k}) q_\ell(-\boldsymbol{k}), \tag{2}$$

where $h_\ell(\boldsymbol{k})$ is defined for $\boldsymbol{k} \in [-\pi/\Delta x, \pi/\Delta x]^d$ with $h_\ell(\boldsymbol{k}) > 0$. We introduced the factor $(\Delta k/2\pi)^d$ considering that $\sum_{\boldsymbol{k}} (\Delta k/2\pi)^d \to \int \mathrm{d}\boldsymbol{k}/(2\pi)^d$ in the limit $\Delta k \to 0$. Note that the Hamiltonian is defined for arbitrary possible ν once $h_\ell(\boldsymbol{k})$ is fixed. The probability density function (PDF) $\rho(\{q\})$ for the microcanonical ensemble with energy E is given by

$$\rho(\{q\}) = \frac{1}{\Omega(E)} \delta\left(H(\{q\}) - E\right), \tag{3}$$

$$\Omega(E) = J \int \mathrm{d}\{q\}\, \delta\left(H(\{q\}) - E\right), \tag{4}$$

where $\delta(\cdot)$ is the Dirac delta function, $\mathrm{d}\{q\} = \prod_{\boldsymbol{k}\in\mathcal{K},\ell} \mathrm{d}\left[\mathrm{Re}\, q_\ell(\boldsymbol{k})\right] \mathrm{d}\left[\mathrm{Im}\, q_\ell(\boldsymbol{k})\right]$ and the factor $J = |\partial\hat{q}_\ell(\boldsymbol{x})/\partial[\mathrm{Re}\, q_{\ell'}(\boldsymbol{k}), \mathrm{Im}\, q_{\ell'}(\boldsymbol{k})]| = (\Delta k/2\pi)^{d\nu/2}[(\Delta x)^d/2]^{-\nu/2}$ is the Jacobian of the Fourier transform. Let the average of a function of state $F(\{q\})$ over the microcanonical ensemble be denoted by $\langle F(\{q\})\rangle$, i.e.

$$\langle F(\{q\})\rangle = J \int d\{q\} \rho(\{q\}) F(\{q\}). \tag{5}$$

A function of state $F(\{q\})$ which is invariant under the spatial translation $\hat{q}_\ell(\boldsymbol{x}) \to \hat{q}_\ell(\boldsymbol{x} - \boldsymbol{n}\Delta x)$ or $q_\ell(\boldsymbol{k}) \to \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{n}\Delta x} q_\ell(\boldsymbol{k})$ with $\boldsymbol{n}$ being a vector with integer components can be given in general by

$$F(\{q\}) = F^{(0)} + \sum_{j=1}^{\infty} F^{(j)}(\{q\}), \tag{6}$$

$$F^{(j)}(\{q\}) = \sum_{\substack{\boldsymbol{k}_1,\cdots,\boldsymbol{k}_j \\ \ell_1,\cdots,\ell_j}} \left(\frac{\Delta k}{2\pi}\right)^{jd} \left(\frac{\Delta k}{2\pi}\right)^{-d} \delta_{\sum_{m=1}^{j} \boldsymbol{k}_m} \times f^{(j)}_{\ell_1\cdots\ell_j}(\boldsymbol{k}_1, \cdots, \boldsymbol{k}_j) \prod_{m'=1}^{j} q_{\ell_{m'}}(\boldsymbol{k}_{m'}), \tag{7}$$

where $F^{(0)}$ is a constant in $\{q\}$, and $\delta_{\boldsymbol{k}}$ is 1 for $\boldsymbol{k} = \boldsymbol{0}$ and 0 otherwise. We introduced the factor $(\Delta k/2\pi)^{-d}$ in Eq. (7) considering that $(\Delta k/2\pi)^{-d}\delta_{\boldsymbol{k}} \to (2\pi)^d\delta(\boldsymbol{k})$ in the limit

$\Delta k \to 0$. Let the function $f^{(j)}_{\ell_1\cdots\ell_j}(\boldsymbol{k}_1,\cdots,\boldsymbol{k}_j)$ in Eq. (7) be given as a term or a summation of terms such that they are asymptotically ν-independent function as $\nu\to\infty$ defined for $\boldsymbol{k}_m \in [-\pi/\Delta x, \pi/\Delta x]^d (1\le m\le j)$ possibly multiplied by a number of functions of the form $(\Delta k/2\pi)^{-d}\delta_{\boldsymbol{g}(\boldsymbol{k}_1,\cdots,\boldsymbol{k}_j)}$ and a factor of the form ν^α, where $\boldsymbol{g}(\boldsymbol{k}_1,\cdots,\boldsymbol{k}_j)$ is a d-dimensional vector-valued function whose form differs in the different factors and α is a constant whose value may differ in different terms. Since the ν-dependence of $f^{(j)}_{\ell_1\cdots\ell_j}(\boldsymbol{k}_1,\cdots,\boldsymbol{k}_j)$ is specified, $F(\{q\})$ is defined for states $\{q\}$ of the systems with arbitrary possible ν.

Let $\mathcal{F}$ be the set of functions such that $F(\{q\})\in\mathcal{F}$ if and only if $F(\{q\})$ satisfies the conditions, (F0) it can be written in the form Eq. (6) with Eq. (7) and the ν-dependence noted above, (F1) for every j and $j'(1\le j'\le j)$, the number of the wavevectors $\boldsymbol{k}_{j'}$ satisfying that there exist $\boldsymbol{k}_1\cdots,\boldsymbol{k}_{j'-1},\boldsymbol{k}_{j'+1},\cdots\boldsymbol{k}_j$ and $\ell_1,\cdots,\ell_j$ such that $f^{(j)}_{\ell_1\cdots\ell_j}(\boldsymbol{k}_1,\cdots,\boldsymbol{k}_{j'},\cdots\boldsymbol{k}_j)\neq 0$ is $O(\nu)$ unless $F^{(j)}(\{q\})=0$, (F2) $F^{(j)}(\{q\})=0$ when j is odd. It can be shown that, for $F(\{q\})\in\mathcal{F}$, the relative variance $(\Delta F)^2/\langle F(\{q\})\rangle^2$ is $O(\nu^{-1})$ in the thermodynamic limit $\nu\to\infty$ with fixed E/ν, where $(\Delta F)^2=\langle[F(\{q\})-\langle F(\{q\})\rangle]^2\rangle$.

The proof is as follows. By substituting the formula

$$\delta(X)=\int_{-\infty}^{\infty}\frac{\mathrm{d}\lambda}{2\pi}\mathrm{e}^{(\epsilon-\mathrm{i}\lambda)X}\qquad(\epsilon>0)\tag{8}$$

into Eq. (4) and using the formula

$$\int_{-\infty}^{\infty}\frac{\mathrm{d}\lambda}{2\pi}\frac{\mathrm{e}^{(\epsilon-\mathrm{i}\lambda)X}}{(\epsilon-\mathrm{i}\lambda)^n}=\frac{X^{n-1}}{(n-1)!}\qquad(\epsilon>0,X>0),\tag{9}$$

where n is a positive integer, we have

$$\Omega(E)=\pi^{\frac{\nu}{2}}(\Delta x)^{-\frac{d\nu}{2}}\frac{E^{\frac{\nu}{2}-1}}{(\frac{\nu}{2}-1)!}\prod_{\boldsymbol{k}\in\mathcal{K},\ell}\big(h_\ell(\boldsymbol{k})\big)^{-1}.\tag{10}$$

We also have

$$\begin{aligned}&\left\langle\prod_{m'=1}^{m}\big(q_{\ell_{m'}}(\boldsymbol{k}_{m'})\,q_{\ell_{m'}}(-\boldsymbol{k}_{m'})\big)^{j_{m'}}\right\rangle\\&=\frac{(\frac{\nu}{2}-1)!}{(\frac{\nu}{2}+j-1)!}\left(\frac{\Delta k}{2\pi}\right)^{-jd}\frac{E^j}{2^j}\\&\quad\times\prod_{m'=1}^{m}\Big[j_{m'}!\big(h_{\ell_{m'}}(\boldsymbol{k}_{m'})\big)^{-j_{m'}}\Big],\end{aligned}\tag{11}$$

where $j=\sum_{m'=1}^{m}j_{m'}$. Note that, if $q_\ell(\boldsymbol{k})$ is not paired with $q_\ell(-\boldsymbol{k})$, the average of the term containing $q_\ell(\boldsymbol{k})$ is 0.

The relative variance can be written as

$$\frac{(\Delta F)^2}{\langle F\rangle^2}=\frac{\sum_{j,j'=0}^{\infty}\Big(\langle F^{(2j)}F^{(2j')}\rangle-\langle F^{(2j)}\rangle\langle F^{(2j')}\rangle\Big)}{\sum_{j,j'=0}^{\infty}\langle F^{(2j)}\rangle\langle F^{(2j')}\rangle},\tag{12}$$

where the condition (F2) is used. Here and hereafter, the arguments $\{q\}$ in $F(\{q\})$ and $F^{(j)}(\{q\})$ are omitted for brevity. There are two types of terms in the numerator of the right hand side of Eq. (12), that are, (i) all the wavevector pairs $(\boldsymbol{k}_m,-\boldsymbol{k}_m)$ in the term are included in either of $F^{(2j)}$ or $F^{(2j')}$, e.g., the term proportional to $f^{(2j)}_{\ell_1\ell_1\cdots\cdots\ell_j\ell_j}(\boldsymbol{k}_1,-\boldsymbol{k}_1,\cdots,\boldsymbol{k}_j,-\boldsymbol{k}_j)$ $f^{(2j')}_{\ell_{j+1}\ell_{j+1}\cdots\ell_{j+j'}\ell_{j+j'}}(\boldsymbol{k}_{j+1},-\boldsymbol{k}_{j+1},\cdots,\boldsymbol{k}_{j+j'},-\boldsymbol{k}_{j+j'})$, and (ii) elements of some wavevector pairs $(\boldsymbol{k}_m,-\boldsymbol{k}_m)$ in the term are contained separately in $F^{(2j)}$ and $F^{(2j')}$, e.g., the term proportional to $f^{(2j)}_{\ell_1\cdots\ell_p\ell_{p+1}\ell_{p+1}\cdots\ell_{j+p/2}\ell_{j+p/2}}(\boldsymbol{k}_1,\cdots,\boldsymbol{k}_p,\boldsymbol{k}_{p+1},-\boldsymbol{k}_{p+1},\cdots,\boldsymbol{k}_{j+p/2},-\boldsymbol{k}_{j+p/2})$ $f^{(2j')}_{\ell_1\cdots\ell_p\ell_{j+p/2+1}\ell_{j+p/2+1}\cdots\ell_{j+j'}\ell_{j+j'}}(-\boldsymbol{k}_1,\cdots,-\boldsymbol{k}_p,\boldsymbol{k}_{j+p/2+1},-\boldsymbol{k}_{j+p/2+1},\cdots,\boldsymbol{k}_{j+j'},-\boldsymbol{k}_{j+j'})$. Each term of type (i) has its counterpart in the denominator of the right hand side of Eq. (12) and the ratio of the term to its counterpart is

$$\frac{(\frac{\nu}{2}+j-1)!\,(\frac{\nu}{2}+j'-1)!}{(\frac{\nu}{2}+j+j'-1)!\,(\frac{\nu}{2}-1)!}=jj'\nu^{-1}+O(\nu^{-2}),\tag{13}$$

which can be shown by using Eq. (11). The terms of type (ii) do not have their counterparts in the denominator and the ratio of the terms to those in the denominator with the same j and j' scale as $O(\nu^0)$ due to the ν-dependence of $f^{(2j)}$ and $f^{(2j')}$. The condition (F0) imposes an extra constraint $\sum_{m=1}^{p} \boldsymbol{k}_m = \boldsymbol{0}$ on wavevectors of the terms of type (ii). The constraint eliminates summation over one wavevector, say $\boldsymbol{k}_1$. Then, from the the condition (F1), the number of the terms of type (ii) is reduces by a factor of $O(\nu)$ in comparison with the terms of type (i) or those in denominators. Thus, the right hand side of Eq. (12) is $O(\nu^{-1})$. This ends the proof.

With the use of Chebyshev's inequality, the probability such that $|F(\{q\}) - \langle F\rangle| > \epsilon|\langle F\rangle|$ is bounded from above by a term scaling as $\epsilon^{-2}O(\nu^{-1})$ for arbitrary $\epsilon > 0$. In this sense, for almost all states $\{q\}$, denoted as typical states, in a microcanonical ensemble, $F(\{q\})$ is almost equal to the microcanonical ensemble average $\langle F\rangle$ for $F \in \mathcal{F}$ and $\nu \gg 1$. The statement implies typicality in the classical system.

Conceptually, the conditions (F0) and (F1) are introduced to restrict the functions of state to those appropriately representing macroscopic variables. When the Hamiltonian is invariant under the spatial translation, field variables summed over spatial coordinates, such as $\sum_{\boldsymbol{x}}(\Delta x)^d \hat{q}_\ell(\boldsymbol{x})$ or $\sum_{\boldsymbol{x}}(\Delta x)^d \hat{q}_\ell(\boldsymbol{x}+\boldsymbol{r})\hat{q}_\ell(\boldsymbol{x})$, may be regarded as natural macroscopic quantities. Since spatially summed quantities are invariant under spatial translations of the field, it seems to be appropriate to require the condition (F0) for the functions of state representing macroscopic variables. The condition (F1) is imposed in order to exclude functions of state such that only few modes $(\boldsymbol{k}, \ell)$ are involved, e.g. $\sum_{(\boldsymbol{k},\ell)\in\mathcal{L}}(\Delta k/2\pi)^d q_\ell(\boldsymbol{k}) q_\ell(-\boldsymbol{k})$ where the size of the set $\mathcal{L}$ is much smaller than ν. The condition (F2) is introduced for the sake of simplicity in the proof. It is expected that the condition would be relaxed in same way.

2 Statewise entropy

By virtue of the typicality, for functions $F \in \mathcal{F}$ and typical states $\{q\}$, $F(\{q\})$ can be regarded as a quantity characterizing the microcanonical ensemble that $\{q\}$ belongs to. Since each microcanonical ensemble corresponds to a thermal equilibrium state specified by the value of energy E in thermodynamics, $F(\{q\})$ is characterizing the thermal equilibrium state that the microcanonical ensemble corresponds to. Recall that all the thermodynamical information of the system is contained in the entropy $S(E)$ as a function of energy E. Then, the function $S(\{q\}) \in \mathcal{F}$ that corresponds to the entropy $S(E)$ is of vital importance from the thermodynamical point of view.

In the following, we construct the statewise entropy $S(\{q\}) \in \mathcal{F}$ that satisfies $\langle S(\{q\})\rangle = S_{\mathrm{MC}}(E)$, where $S_{\mathrm{MC}}(E) = \ln[\Omega(E)\Delta E]$ is the standard definition of the entropy for the microcanonical ensemble, ΔE is a energy width which scales as $O(E)$ and the unit in which the Boltzmann constant is unity is used. The basic idea of the construction is as follows. In conventional statistical mechanics, the entropy S is defined to an ensemble of states, or in other words, a PDF on the state space. For a single state $\{q\}$, we generate an ensemble of states $\{\chi\}(\{q\}, \boldsymbol{a})(\boldsymbol{a} \in \mathcal{A})$, as will be introduced below, and define the statewise entropy $S(\{q\})$ to the PDF of $\{\chi\}(\{q\}, \boldsymbol{a})$ by analogy with the conventional statistical mechanics.

For a state $\{q\}$, we introduce shifted states $\{\chi\}(\{q\}, \boldsymbol{a})$ in wavevector space as

$$\chi_\ell(\boldsymbol{k}, \{q\}, \boldsymbol{a}) = \begin{cases} q_\ell(\boldsymbol{k}+\boldsymbol{a}) \left(\frac{\Delta k}{2\pi}\right)^{\frac{d}{2}} & ((\boldsymbol{k} \in \mathcal{K}) \wedge (\boldsymbol{k}+\boldsymbol{a} \in \mathcal{K})) \\ q_\ell(\boldsymbol{k}-\boldsymbol{a}) \left(\frac{\Delta k}{2\pi}\right)^{\frac{d}{2}} & ((\boldsymbol{k} \in \mathcal{K}^-) \wedge (\boldsymbol{k}-\boldsymbol{a} \in \mathcal{K}^-)) \\ 0 & (\text{otherwise}) \end{cases}, \tag{14}$$

where $\mathcal{K}^- = \{\boldsymbol{k}| - \boldsymbol{k} \in \mathcal{K}\}$, $\boldsymbol{a} \in \mathcal{A}$ and $\mathcal{A} = \{\boldsymbol{a}|\boldsymbol{a} = (n_1\Delta k, \cdots, n_d\Delta k)$, $n_i = -\lfloor\zeta N/2\rfloor$, $-\lfloor\zeta N/2\rfloor + 1, \cdots, 0, 1, \cdots, \lfloor\zeta N/2\rfloor - 1\}$ with ζ being a ν-independent constant such that $0 < \zeta \ll 1$. Once ζ is fixed, N is varied in the range $N \gg \zeta^{-1}$. The factor $(\Delta k/2\pi)^{d/2}$ in Eq.(14) is introduced so as the variance $\langle\chi_\ell(\boldsymbol{k}, \{q\})\chi_\ell(-\boldsymbol{k}, \{q\})\rangle$ to scale as $O(\nu^0)$. Let us denote the average over the ensemble of $\boldsymbol{a}$ by $\langle\cdot\rangle_{\boldsymbol{a}}$, i.e.

$$\langle X(\boldsymbol{a})\rangle_{\boldsymbol{a}} = \frac{1}{\lfloor\zeta N\rfloor^d} \sum_{\boldsymbol{a}\in\mathcal{A}} X(\boldsymbol{a}). \tag{15}$$

The moment generating function of $\{|\chi|^2\}(\{q\},\boldsymbol{a})$ with respect to the ensemble of $\boldsymbol{a}$ is given by

$$\begin{aligned}
&\varphi(\{\xi\};\{q\}) \\
&= \left\langle \exp\left[\mathrm{i} \sum_{\boldsymbol{k}\in\mathcal{K},\ell} \left(\frac{\Delta k}{2\pi}\right)^d \xi_\ell(\boldsymbol{k})\, |\chi_\ell(\boldsymbol{k},\{q\},\boldsymbol{a})|^2 \right] \right\rangle_{\boldsymbol{a}} \\
&= 1 + \sum_{j=1}^{\infty} \left[\sum_{\substack{\boldsymbol{k}_1,\cdots \boldsymbol{k}_{2j} \\ \ell_1\cdots\ell_{2j}}} \left(\frac{\Delta k}{2\pi}\right)^{(2j-1)d} \delta_{\sum_{m=1}^{2j} \boldsymbol{k}_m} \right. \\
&\qquad \left. \times\, \varphi^{(2j)}_{\ell_1\cdots\ell_{2j}}(\{\xi\};\boldsymbol{k}_1,\cdots,\boldsymbol{k}_{2j}) \prod_{m'=1}^{2j} q_{\ell_{m'}}(\boldsymbol{k}_{m'}) \right],
\end{aligned} \tag{16}$$

where

$$\begin{aligned}
&\varphi^{(2j)}_{\ell_1\cdots\ell_{2j}}(\{\xi\};\boldsymbol{k}_1,\cdots,\boldsymbol{k}_{2j}) = \frac{\mathrm{i}^j}{j!}\left(\frac{\Delta k}{2\pi}\right)^d \\
&\times \left(\prod_{m=1}^{j-1} \delta_{\boldsymbol{k}_{2m-1}+\boldsymbol{k}_{2m}} \right) \left\langle \prod_{m'=1}^{j} \xi_{\ell_{m'}}(\boldsymbol{k}_{2m'-1}-\boldsymbol{a}) \right\rangle_{\boldsymbol{a}},
\end{aligned} \tag{17}$$

with $\xi_\ell(\boldsymbol{k})$ being a real function of $\boldsymbol{k}=(k_1,\cdots,k_d)$ with $k_1\in[0,\pi/\Delta x), k_i\in[-\pi/\Delta x,\pi/\Delta x)$ $(i=2,\cdots d)$ and $\xi_\ell(\boldsymbol{k})=0$ otherwise. Let $\xi_\ell(\boldsymbol{k})$ be given as a term or a summation of terms such that they are ν-independent functions or functions of the form $B(\Delta k/2\pi)^{-d}\delta_{\boldsymbol{k}-\boldsymbol{K}}$ multiplied by a factor of the form ν^α, where B,α and $\boldsymbol{K}$ are constants whose values may differ in different terms. It can be shown that $\varphi(\{\xi\};\{q\})$ satisfies the condition (F0) for every $\{\xi\}$ by noting that

$$\lim_{\nu\to\infty}\langle X(\boldsymbol{a})\rangle_{\boldsymbol{a}} = \left(\frac{\Delta x}{\zeta}\right)^d \int_{[-\zeta\pi/\Delta x,\zeta\pi/\Delta x)^d} \frac{\mathrm{d}\boldsymbol{a}}{(2\pi)^d} X(\boldsymbol{a}), \tag{18}$$

for a ν-independent function $X(\boldsymbol{a})$. It is evident that (F2) is satisfied for $\varphi(\{\xi\};\{q\})$ with every $\{\xi\}$. When $\xi_\ell(\boldsymbol{k})=(\Delta k/2\pi)^{-d}\delta_{\boldsymbol{k}-\boldsymbol{K}}\delta_{\ell\ell_0}$, we see that (F1) is satisfied since $\varphi^{(2j)}_{\ell_1\cdots\ell_{2j}}(\{\xi\};\boldsymbol{k}_1,\cdots,\boldsymbol{k}_{2j})\neq 0$ for $\boldsymbol{k}_{2m-1}=-\boldsymbol{k}_{2m}=\boldsymbol{K}+\boldsymbol{a}$ $(m=1,\cdots,j)$ with $\boldsymbol{a}\in\mathcal{A}$ and $\ell_m=\ell_0(m=1,\cdots,2j)$. This example suffices to show that (F1) is satisfied for $\varphi(\{\xi\};\{q\})$ with every $\{\xi\}$. Consequently, we have $\varphi(\{\xi\};\{q\})\in\mathcal{F}$ for every $\{\xi\}$.

For every fixed $\{q\}$, the PDF of $\{|\chi|^2\}(\{q\},\boldsymbol{a})$ with respect to the ensemble of $\boldsymbol{a}$, which is denoted by $P_2(\{|\chi|^2\};\{q\})$, is given by the inverse Fourier transform of $\varphi(\{\xi\};\{q\})$, i.e.

$$\begin{aligned}
&P_2(\{|\chi|^2\};\{q\}) = \left(\frac{\Delta k}{2\pi}\right)^{\frac{d\nu}{2}} \int \frac{\mathrm{d}\{\xi\}}{(2\pi)^{\frac{\nu}{2}}} \\
&\times \exp\left\{ \sum_{\boldsymbol{k}\in\mathcal{K},\ell} \left[-\mathrm{i}\left(\frac{\Delta k}{2\pi}\right)^d \xi_\ell(\boldsymbol{k})|\chi_\ell(\boldsymbol{k})|^2 \right.\right. \\
&\qquad \left.\left. -\frac{1}{2}\left(\frac{\Delta k}{2\pi}\right)^{2d} (\xi_\ell(\boldsymbol{k}))^2\sigma^2 \right] \right\} \varphi(\{\xi\};\{q\}),
\end{aligned} \tag{19}$$

where $\sigma>0$ is introduced for the regularization of the PDF that is otherwise an ensemble of Dirac delta functions. The PDF, $P(\{\chi\};\{q\})$, of $\{\chi\}(\{q\},\boldsymbol{a})$ with respect to the ensemble of $\boldsymbol{a}$, which is consistent with $P_2(\{|\chi|^2\};\{q\})$ and independent of $\{\arg\chi\}$, is given by

$$P(\{\chi\};\{q\}) = \frac{1}{\pi^{\frac{\nu}{2}}} P_2(\{|\chi|^2\};\{q\}). \tag{20}$$

Let us define the statewise entropy by

$$S(\{q\}) = -\int \mathrm{d}\{\chi\} P(\{\chi\};\{q\}) \ln P(\{\chi\};\{q\}). \tag{21}$$

It can be shown that $P_2(\{|\chi|^2\};\{q\}), P(\{\chi\};\{q\})\in\mathcal{F}$ for every $\{\chi\}$ and $S(\{q\})\in\mathcal{F}$ by expanding them into the Maclaurin series with respect to $\{q\}$. Therefore, $S(\{q\})$ is almost equal to $\langle S(\{q\})\rangle$ for typical states $\{q\}$ in the microcanonical ensemble.

The average of $\varphi(\{\xi\};\{q\})$ over the microcanonical ensemble is given by

$$\langle\varphi(\{\xi\};\{q\})\rangle \approx \left\langle \prod_{\boldsymbol{k}\in\mathcal{K},\ell}\left(1-\mathrm{i}\frac{E}{\nu}\left(\frac{\Delta k}{2\pi}\right)^d\frac{\xi_\ell(\boldsymbol{k}-\boldsymbol{a})}{h_\ell(\boldsymbol{k})}\right)^{-1}\right\rangle_{\boldsymbol{a}}$$
$$\approx \prod_{\boldsymbol{k}\in\mathcal{K},\ell}\left(1-\mathrm{i}\frac{E}{\nu}\left(\frac{\Delta k}{2\pi}\right)^d\frac{\xi_\ell(\boldsymbol{k})}{h_\ell(\boldsymbol{k})}\right)^{-1}, \tag{22}$$

where, in the first line, Eq. (9) and $\nu \gg 1$ are used, and, in the second line, the change of the variable $\boldsymbol{k}\to\boldsymbol{k}+\boldsymbol{a}$ is applied with neglecting the effect of wavevectors such that $\boldsymbol{k}\pm\boldsymbol{a}\notin\mathcal{K}$, the ratio of whose number to the total number of wavevectors in $\mathcal{K}$ is $O(\zeta)$, and $h_\ell(\boldsymbol{k})$ is assumed to be smooth so that $h_\ell(\boldsymbol{k}+\boldsymbol{a})\approx h_\ell(\boldsymbol{k})$ with $|\boldsymbol{a}|=O(\zeta)$. It follows that

$$\langle P(\{\chi\};\{q\})\rangle = \prod_{\boldsymbol{k}\in\mathcal{K},\ell}\left(\frac{1}{\pi}\frac{\nu}{E}h_\ell(\boldsymbol{k})\mathrm{e}^{-\frac{\nu}{E}h_\ell|\chi_\ell(\boldsymbol{k})|^2}\right), \tag{23}$$

where we took the limit $\sigma\to 0$ after taking the ensemble average over the microcanonical ensemble and using $\nu\gg 1$ for Eq. (19). We finally obtain

$$\langle S(\{q\})\rangle \approx -\int \mathrm{d}\{\chi\}\,\langle P(\{\chi\};\{q\})\rangle \ln\langle P(\{\chi\};\{q\})\rangle$$
$$= \frac{\nu}{2}\ln\left(\pi\mathrm{e}\frac{E}{\nu}\right) - \sum_{\boldsymbol{k}\in\mathcal{K},\ell}\ln h_\ell(\boldsymbol{k}). \tag{24}$$

Note that we can add an arbitrary term of the form $C\nu$, where C is a constant, to the definition of the entropy without changing the thermodynamical properties of the system. By adding $-(\nu/2)\ln[(\Delta x)^d/2]$, the second line of (24) coincides with the result from the standard definition of entropy $S_{\mathrm{MC}}(E)$ with Eq. (4).

We have constructed the statewise entropy $S(\{q\})$ whose value almost coincide with the standard entropy $S_{\mathrm{MC}}(E)$ for typical states $\{q\}$ in the system of an ensemble of classical harmonic oscillators. Note that the shifted states in the wavevector space $\{\chi\}(\{q\},\boldsymbol{a})$ are auxiliary states for the formal construction of $S(\{q\})$ and they need not be realized physically. One interpretation of employing the shifted states can be given as follows. Note that

$$\langle q_\ell(\boldsymbol{k})q_{\ell'}(-\boldsymbol{k}')\rangle = \frac{E}{\nu h_\ell(\boldsymbol{k})}\left(\frac{\Delta k}{2\pi}\right)^{-d}\delta_{\boldsymbol{k}-\boldsymbol{k}'}\delta_{\ell\ell'}, \tag{25}$$

which is a special case of Eq.(11) with the subsequent sentence. Eq.(25) implies that, as far as the second order moments are concerned, $q_\ell(\boldsymbol{k})$ and $q_\ell(\boldsymbol{k}')$ are uncorrelated for $\boldsymbol{k}\neq\boldsymbol{k}'$ and they have similar value of moments for $\boldsymbol{k}\approx\boldsymbol{k}'$ considering $h_\ell(\boldsymbol{k})\approx h_\ell(\boldsymbol{k}')$. Then, it is tempting to use an ensemble of $q_\ell(\boldsymbol{k})$ generated by fixing a state $\{q\}$ and varying $\boldsymbol{k}$ around $\boldsymbol{k}_0$ as a substitute of the ensemble generated by varying states $\{q\}$ and fixing $\boldsymbol{k}=\boldsymbol{k}_0$.

We used the Hamiltonian $H(\{q\})$ only to specify the value of the energy and no information of $H(\{q\})$ as the generator of time evolution is used. Therefore, $S(\{q\})$ has nothing to do with any kind of time averaging.

States $\{q\}$ with atypical value of $S(\{q\})$ are rare but do exist. It is expected that they are regarded as nonequilibrium states. Although the meaning of $S(\{q\})$ for nonequilibrium states is not clear yet in the context of thermodynamics, we can formally obtain the time evolution of $S(\{q\})$ from a single trajectory in the state space. Unlike conventional definitions of entropy, an ensemble of trajectories or time evolution of a PDF in the state space is not necessary. Furthermore, since the total system is not divided into a subsystem and the bath, we can discuss the time evolution of $S(\{q\})$ in isolated systems. However, in order to study the redistribution of energy among different wavevector modes, that is essential in time evolution of nonequilibrium processes, possibly small but nonzero interaction terms among different wavevectors, which are higher order in $\{q\}$ and neglected in Eq. (2), are necessary.

Let us see the statewise entropy $S(\{q\})$ in a simple example of a nonequilibrium state and a nonequilibrium process. We consider the case that the Hamiltonian of the system is given by $H^{(1)}$ for time $t<t_0$ and $H^{(2)}$ for time $t\geq t_0$, where $H^{(i)}$ are specified by $h_\ell^{(i)}(\boldsymbol{k})(i=1,2)$ in Eq.(2). Let the system be macroscopically at the thermal equilibrium

state of energy $E^{(1)}$ for $t < t^{(1)}$. We assume that the Hamiltonian is suddenly changed at $t = t^{(1)}$ without changing the microscopic state $\{q(t^{(1)})\}$. Then, the energy of the system is typically changed to $E^{(2)} = \langle H^{(2)} \rangle^{(1)}_{E^{(1)}}$, where $\langle F \rangle^{(i)}_{E}$ denotes the ensemble average of $F(\{q\})$ over the microcanonical ensemble specified by $H^{(i)} = E$. It is expected that the system becomes nonequilibrium with the change of the Hamiltonian at $t = t_1$ and that the system reaches a new thermal equilibrium state after a sufficiently long time, say at $t = t^{(2)}$, through a non-quasistatic, i.e. nonequilibrium, adiabatic process in the presence of small but nonzero interaction terms among different wavevectors. Since the statewise entropy $S(\{q\})$ is defined for states without referring to the Hamiltonian, we typically have $S(\{q(t^{(1)})\}) = S^{(1)}_{\mathrm{MC}}(E^{(1)})$. It can be checked that $S^{(2)}_{\mathrm{MC}}(E^{(2)}) \geq S^{(1)}_{\mathrm{MC}}(E^{(1)})$, where the equality holds when $h^{(2)}_{\ell}(\boldsymbol{k})/h^{(1)}_{\ell}(\boldsymbol{k})$ is constant in $\boldsymbol{k}$ and ℓ. Hence, we typically have $S(\{q(t^{(2)})\}) \geq S(\{q(t^{(1)})\})$ for the non-quasistatic adiabatic process. The result is consistent with the conventional thermodynamics.

It would be a future study to extend the present results, the proof of typicality and the construction of statewise entropy, to classical systems whose Hamiltonians have the higher order terms. Although typicality for quantum systems has already been discussed in a general framework in Refs. [1, 2, 3, 4], the subject would be studied from a new aspect by applying the present field-theoretical formalism to quantum systems.

acknowledgments

The author thanks Yasuhiro Tokura for discussion. The author also thanks the anonymous referee for valuable comments on the earlier version of this letter.

References

[1] Sugita A., *RIMS Kokyuroku (Kyoto)* **1507**(2006) 147.

[2] Sugita A., *Nonlinear Phenomena in Complex Systems* **10**(2007) 192.

[3] Popescu S., Short A. J. and Winter A.,*Nature Physics* **2**(2006) 754.

[4] Goldstein S., Lebowitz J. L., Tumulka R. and Zanghì N., *Physical Review Letters* **96**(2006) 050403.

[5] Plastino A. R. and Daffertshofer A., *EPL* **84**(2008) 30006.