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Stochastic deformation of a thermodynamic symplectic structure

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A stochastic deformation of a thermodynamic symplectic structure is studied. The stochastic deformation is analogous to the deformation of an algebra of observables such as deformation quantization, but for an imaginary deformation parameter (the Planck constant). Gauge symmetries of thermodynamics and corresponding stochastic mechanics, which describes fluctuations of a thermodynamic system, are revealed and gauge fields are introduced. A physical interpretation to the gauge transformations and gauge fields is given. An application of the formalism to a description of systems with distributed parameters in a local thermodynamic equilibrium is considered.

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I. INTRODUCTION

A geometric description of thermodynamic systems has a long history and was initiated by Gibbs [1]. In this approach, equations of state of a thermodynamic system are represented by a surface in a space of thermodynamic parameters. Later this geometric formalism was developed in the works [2–5] on axiomatic foundations of thermodynamics, where its laws were formulated in terms of differential forms. Due to Hermann [6], symplectic and contact geometries acquire a distinctive form in thermodynamics, though some elements of these geometries were introduced by Gibbs as well. Notions of symplectic, contact, Riemannian, and Finslerian geometries in thermodynamics get a further development in Refs. [7–15]. Since the symplectic structure arose, a strong analogy of thermodynamics with classical mechanics and optics was understood soon afterwards [16–22]. Thermodynamics was realized as a Hamiltonian dynamical system. The next logical step is to "quantize" such a dynamical system in order to describe its fluctuations, as it was posed in [17]. At the same time this "quantization" is not a quantal one, which is given in [22], but has to result in a Fokker-Planck-type equation for a probability distribution of thermodynamic variables. The inverse procedure of "dequantization" (the weak noise limit) of the Fokker-Planck equation is of common knowledge [23–25] and also endows thermodynamics with the symplectic structure. In this paper, we shall see that the desired "quantization" is a stochastic deformation procedure proposed in [26], which is an analog of the algebraic approach to quantization known as deformation quantization [27–30].

A theory of fluctuations of thermodynamic quantities is well-known both for equilibrium [31] and nonequilibrium processes, and has a huge literature (see, e.g., [24,32–40]). Thus the aim of "quantization" lies in a construction of stochastic mechanics[1] by means of a procedure similar to an ordinary quantization, while it should give rise to the standard theory of fluctuations and be equivalent to operator methods of stochastic mechanics [42–45]. Stochastic deformation applied to thermodynamics complies with these requirements and reproduces known operator methods in some particular gauges. Gauge transformations and gauge fields are necessary ingredients of stochastic deformation. Furthermore, as we shall see, they are intrinsic to thermodynamics. Transformations of this kind arise occasionally in the literature [25,46] as some tricks to prove, for example, an equivalence of the Doi [47–50] and Martin-Siggia-Rose [42,51–55] formalisms [56], or to establish certain properties of the operator's spectrum of the master equation, or they appear in the form of nonstandard inner products [24,37,57], or as the α degree of freedom in Umezawa's thermo field dynamics [58], and so on. As long as thermodynamics and stochastic mechanics have such symmetries, it is of importance to represent their governing equations in an explicitly invariant form such as, for example, representing the Maxwell equations in an explicitly Lorentz and gauge covariant fashion.

Stochastic deformation of the thermodynamic symplectic structure reveals, first, a perfect analogy of thermodynamics and stochastic mechanics on the one hand with classical mechanics and its quantum deformation on the other hand. Second, it allows us to discover natural gauge structures of thermodynamics and stochastic mechanics and formulate them in gauge invariant forms. In comparison with the standard operator approach to stochastic mechanics, we effectively introduce an additional Stückelberg field and corresponding gauge fields, which result in gauge invariant dynamics. A significant feature of these rather formal manipulations is that the Stückelberg field possesses a physical interpretation. It is an entropy of the thermodynamic system, while the gauge fields are external thermodynamic forces acting on it.

It is worthwhile to mention the works that are intimately related to the subject matter of the present paper. A probabilistic stochastic deformation of a linear symplectic structure was studied in Ref. [59] within the framework of Zambrini's Euclidean quantum mechanics [60,61]. The latter stems from Schrödinger's works [62] made in attempt to give a stochastic interpretation to quantum mechanics. In Ref. [63], Lagrangian and Hamiltonian descriptions of Smoluchowski diffusion processes are given as a special case of the general formalism based on diffusion-type equations. Notice also that something similar to the gauge fields we are about to consider arose in [38]. Gauge transformations, but of a dif-

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[1] To avoid misunderstanding, we point out that we use the term "stochastic mechanics" in a general sense like a notion that unifies various physical models with dynamics obeying some kind of master equation. It is not Nelson's stochastic mechanics [41].

ferent type, were introduced into thermodynamics in [12].

The paper is organized as follows. We start with a formulation of thermodynamics in terms of symplectic geometry (Sec. II). Then we realize nonequilibrium thermodynamics as a certain Hamiltonian dynamical system and establish its gauge invariance. Here we also introduce gauge fields and provide their physical interpretation. In Sec. III, we consider a stochastic deformation of the obtained Hamiltonian dynamical system and investigate some of its properties. We introduce an operator of dissipation, which is the stochastic analog of a dissipation function [34], and express an entropy production through it. As an example we apply the formalism to a thermodynamic system being in a local thermodynamic equilibrium. In conclusion, we outline the prospects for further generalizations and research. We assume Einstein's summation rule unless otherwise stated. Latin indices run from 1 to d, where d is a number of extensive variables, and zero index corresponds to time.

II. THERMODYNAMICS

All the statistical properties of a quantum system in a thermostat are determined by the partition function

$$Z(p_1, \ldots, p_{d-1}, x^d) := \operatorname{Tr} \exp\left(-\sum_{i=1}^{d-1} p_i \hat{x}^i\right), \tag{1}$$

where $\hat{x}^i$ are quantum operators of additive integrals of motion, x^d is some fixed extensive variable, for instance, the volume, and p_i are intensive parameters thermodynamically conjugate to $\hat{x}^i$ or thermodynamic forces. The Hamiltonian and the reciprocal temperature are among these conjugate pairs. Differentiating the partition function with respect to p_i and making the Legendre transform, we arrive at the first law of thermodynamics,

$$dS(x) = p_i dx^i, \tag{2}$$

where x^i are averages of the corresponding operators, $S(x)$ is the entropy of the system, which is the Legendre transform of the Massieu function [5] $\Phi := -\ln Z$, and we introduce the intensive parameter $p_d := \partial_d S(x)$ conjugate to x^d. In geometric terms, the first law (2) endows the space of states (x,p) of a thermodynamic system with a symplectic structure specified by the symplectic potential $\theta := p_i dx^i - dS$. According to Eq. (2), the system is confined to the Lagrangian surface of the symplectic 2-form $d\theta$. Inversely, any Lagrangian surface uniquely projectable to the space of extensive variables $\{x^i\}$ can be locally represented by the equality of the form (2) (see, e.g., [18]). For reasonable physical systems, the Lagrangian surface is uniquely projectable, otherwise a change of thermodynamic forces does not vary extensive parameters, that is, we have a system with zero (generalized) compressibility.

In nonequilibrium with the thermostat, the thermodynamic system moves along the Lagrangian surface. Besides, if we directly (not by means of intensive parameters) change the entropy of the system, the Lagrangian surface (2) also evolves. A natural generalization of the first law to nonequilibrium processes looks like

$$dS(t,x) = p_i dx^i - H(x,p,t)dt, \tag{3}$$

where $H(x,p,t)$ is a thermodynamic force conjugate to time or the Hamilton function.[2] The Hamilton function taken on the Lagrangian surface is a source of the entropy and it vanishes if the functional form of the entropy does not change. The nonstationary first law (3) represents the Hamilton-Jacobi equation. It is valid when it is reasonable to attribute certain values of intensive parameters to the whole thermodynamic system.

The requirement that the system should be confined to the Lagrangian surface restricts the form of the Hamilton function. Here we consider two equivalent mechanisms for how to keep the system on the Lagrangian surface,

$$T_i := p_i - \partial_i S = 0. \tag{4}$$

The first one is a "rigid" method. We demand that T_i are integrals of motion of the Hamilton system associated with Eq. (3). A general form of a regular in momenta Hamilton function meeting this requirement is

$$H = c(t) - \partial_t S + T_i v^i(t,x) + \frac{1}{2} T_i g^{ij}(t,x) T_j + \cdots, \tag{5}$$

where v^i and $g^{ij} = g^{ji}$ are some contravariant tensors, dots denote the terms of higher order in T_i, and $c(t)$ is some function. Redefining the entropy, we eliminate the latter function. Then for a stationary entropy, the Hamilton function (5) is zero on the Lagrangian surface. The Hamilton equations of motion of the thermodynamic system become

$$\dot{x}^i = \{x^i, H\} \approx v^i, \quad \dot{T}_i = \partial_t T_i + \{T_i, H\} \approx 0, \tag{6}$$

where curly brackets denote the Poisson brackets, and approximate equalities mean that we take equations on the Lagrangian surface (4). Now we see that the vector field v^i describes a drift of the system. The tensor g^{ij} and higher terms in the expansion (5) gain a physical meaning only upon stochastic deformation of the Hamiltonian system, which will be considered below. They are responsible for a probability distribution law of fluctuations of statistical averages.

The Hamiltonian action functional associated with (3) is obvious. If the expansion of the Hamilton function (5) terminates at the term quadratic in T_i and the tensor g^{ij} is nondegenerate, it is not difficult to obtain a Lagrangian form of this action,

$$S[x(t)] = \int dt \left[\frac{1}{2} g_{ij} (\dot{x}^i - v^i)(\dot{x}^j - v^j) + \frac{dS}{dt}\right], \tag{7}$$

where g_{ij} is the inverse of g^{ij}. This functional is the well-known Onsager-Machlup action [34–36]. It measures an entropy change along a trajectory $x(t)$. The first term measures an additional entropy production caused by fluctuations deviating intensive parameters of the system from the Lagrangian surface. This term vanishes in the thermodynamic limit

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[2] Of course, this Hamilton function is not related, at least immediately, to the Hamiltonian entering the partition function (1). In [39,40] this thermodynamic force is called the kinetic potential.

(6). The second term is a change of the thermodynamic entropy. The principle of least action corresponding to Eq. (7) says that the system moves to equilibrium with a minimum of the entropy production. Therefore, the first term has to be non-negative for an arbitrary trajectory and the tensor g^{ij} must be positive definite. Further, if the fluctuations are described by a general Markov process, it can be proven [40] that $\partial^{ij}_p H$ should be positive definite.

Under the above restrictions on g^{ij}, any drift vector field can be represented in the form

$$v^i = g^{ij}(\partial_j S - A_j), \tag{8}$$

where $A_i(t,x)$ is some local 1-form, which we shall call the gauge field. The quantity in the brackets is the total thermodynamic force, while the gauge field A_i is the external force exerting on the system. In particular, the Onsager principle [32] postulates the drift (8) and that the thermostat acts on the nonequilibrium system as

$$A_i(t,x) = \partial_i S(t,x_0), \tag{9}$$

where x_0^i is the solution of Eq. (4) at fixed intensive parameters p_i characterizing the thermostat. To provide a stability of the state x_0 of the system, we have to require a negative definiteness of the Hessian $\partial_{ij}S(x_0)$, otherwise the system is in a phase transition state. If the total thermodynamic force is given, the relation (8) can be only a linear approximation to a nonlinear response of the system to the uncompensated force. Besides, there are systems that do not obey the Onsager principle (see, for physical examples, [24,33,45,53]).

The first law (3) with the Hamilton function (5) is invariant under the following gauge transformations:

$$p_i \to p_i + \partial_i \xi(t,x), \quad A_i \to A_i + \partial_i \xi(t,x),$$

$$S(t,x) \to S(t,x) + \xi(t,x). \tag{10}$$

Their existence reflects the fact that a gradient part of the external force can be attributed to the system itself redefining its entropy. In other words, these transformations relate equivalent thermodynamic systems (system)+(thermostat). They are not distinguishable within thermodynamics since the total forces do not change under the gauge transformations (10).

Now we are in a position to introduce the second method to confine the system to the Lagrangian surface. This method is, of course, equivalent to the first one and based on using an auxiliary compensating field. We postulate that the first law (3) is invariant under the gauge transformations (10). In addition, we seek the Hamilton function, which does not depend on the entropy. Then a quadratic in momenta Hamilton function[3] providing gauge invariance to Eq. (3) can be cast into the form of the Hamilton function of a charged particle in an electromagnetic field,

$$H = \frac{1}{2}\mathcal{P}_i g^{ij}\mathcal{P}_j - A_0 =: K(p,x) - A_0, \quad \mathcal{P}_i := p_i - A_i, \tag{11}$$

where $A_0(t,x)$ is the auxiliary field transforming under the gauge transformations as

$$A_0 \to A_0 + \partial_t \xi(t,x). \tag{12}$$

It keeps an invariance of Eq. (3) with respect to nonstationary gauge transformations. To confine the system to the Lagrangian surface determined by a given entropy function $S(t,x)$, we have to choose the compensating field A_0 so that the Hamilton-Jacobi equation is fulfilled,

$$A_0 - \partial_t S = \frac{1}{2} g^{ij}(\partial_i S - A_i)(\partial_j S - A_j). \tag{13}$$

If we substitute A_0 from the Hamilton-Jacobi equation to the Hamilton function (11), we revert to Eq. (5) with the drift vector field (8) establishing the equivalence of two approaches. The gauge invariant total force $A_0 - \partial_t S$ is the kinetic part K of the Hamilton function taken on the Lagrangian surface. These two functions, $A_0 - \partial_t S$ and K, are different representations of the dissipative function $\Psi(X,X)$ introduced in [34]. The entropy production $\dot{\Sigma}$ in the whole system (thermostat)+(system) is standardly expressed in terms of the dissipation function

$$\dot{\Sigma} \approx \mathcal{P}_i \frac{\partial K}{\partial p_i} = 2K, \tag{14}$$

where we assume that the rate of an entropy change of the thermostat is $-v^i A_i$.

Given K and A_μ completely define the system and, in particular, its thermodynamic entropy through the Hamilton-Jacobi equation. From a mechanical viewpoint, a thermodynamic system (11) tends to an unstable equilibrium of the potential $-A_0$. That is, for any given x we take such an initial momentum p that the "particle" hits precisely the equilibrium point with zero velocity. Although this point is unstable equilibrium, it is of course an attractor on the Lagrangian surface. Not any mechanical Hamilton function (11) having a nonstable equilibrium point in its potential can serve as the Hamilton function for some thermodynamic system even in a neighborhood of this point. The "magnetic" field can freeze the particle (such as in a magnetized plasma) so it never reaches the equilibrium. Linearizing the particle's equations of motion in a small vicinity of the stationary point x_0 and assuming that the Hamilton function is stationary and the fields entering it are smooth enough, one finds that for the isotropic potential $\partial_{ij}A_0(x_0) = \xi g_{ij}(x_0)$ the system never hits the point x_0 starting in an arbitrary point of its small vicinity only if

$$|\lambda_i| > 4\xi \tag{15}$$

for some i, where λ_i are the characteristic numbers

$$\det(F_{ik}g^{kl}F_{lj} - \lambda g_{ij}) = 0, \quad F_{ij} := \partial_{[i}A_{j]}(x_0). \tag{16}$$

In other words, the condition (15) reminds us that the gauge fields A_i should enter the potential A_0 according to the Hamilton-Jacobi equation (13).

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[3] A generalization of these considerations to Hamilton functions of an arbitrary order in momenta is straightforward, but has no such suggestive mechanical analogy. Quadratic in momenta, Hamilton functions correspond to a Gaussian distribution law of fluctuations δ-correlated in time.

III. FLUCTUATIONS

Now we turn to fluctuations of statistical averages. As was shown in [26], these fluctuations can be obtained by stochastic deformation of the corresponding Poisson structure. In our case, we shall deform a canonical symplectic structure associated with the thermodynamic system.

Let us briefly recall some basic features of an algebraic stochastic deformation. For more details, an interested reader can consult Ref. [26] and the classical works on deformation quantization [27–30]. A commutative associative algebra of classical observables is constituted by real smooth functions over the symplectic space. We deform this algebra in a manner of deformation quantization, but with an imaginary deformation parameter, such that

$$[\hat{x}^i,\hat{p}_j]=\nu\delta^i_j, \tag{17}$$

where ν is the real positive deformation parameter. Carets signify elements of the deformed associative algebra and we imply the Weyl-Moyal star-product [64],

$$\hat{F}\hat{G}=\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{\nu}{2}\right)^n\omega^{a_1b_1}\ldots\omega^{a_nb_n}\partial_{a_1\cdots a_n}F(z)\partial_{b_1\cdots b_n}G(z), \tag{18}$$

where $z\equiv(x,p)$, $a_n,b_n=\overline{1,2d}$, the functions $F(z)$ and $G(z)$ are the Weyl symbols of the corresponding elements of the deformed algebra, and ω^{ab} is the inverse to the symplectic 2-form ω_{ab}. The generators $\hat{x}^i$ and $\hat{p}_j$ of the Heisenberg-Weyl algebra correspond to extensive and intensive parameters of the thermodynamic system. The deformation parameter ν is not the Planck constant. It characterizes a variance of fluctuations and, as we shall see, is equal to double the Boltzmann constant, $\nu=2k_B$, for thermal fluctuations.

Another necessary ingredient of the deformation procedure is the trace functional Tr, which is a linear functional on the deformed algebra mapping to real numbers and vanishing on commutators. An explicit formula for the trace of an element $\hat{F}$ has the form

$$\mathrm{Tr}\,\hat{F}=\int\frac{d^dxd^dp}{(2\pi\nu)^d}F(x,ip). \tag{19}$$

A state of a stochastic system is characterized by an element $\hat{\rho}$ with a unit trace

$$\mathrm{Tr}\,\hat{\rho}=1. \tag{20}$$

The pure state is specified by an additional idempotency requirement

$$\hat{\rho}^2=\hat{\rho}. \tag{21}$$

An average of some observable $\hat{F}$ over the state $\hat{\rho}$ is defined by the standard formula

$$\langle\hat{F}\rangle\coloneqq\mathrm{Tr}(\hat{\rho}\hat{F}). \tag{22}$$

Thus, for a correct probabilistic interpretation the state $\hat{\rho}$ should satisfy

$$\langle\delta^d(\hat{x}^i-x^i)\rangle\geqslant0,\qquad\forall\ x\in\mathbb{R}^d. \tag{23}$$

The dynamics of the stochastic system in the state $\hat{\rho}$ are generated by the element $\hat{H}$ of the deformed algebra, which corresponds to the Hamilton function $H(t,x,p)$, and obey the von Neumann equation

$$\nu\dot{\hat{\rho}}=[\hat{H},\hat{\rho}]. \tag{24}$$

In the case of a linear symplectic space, it is useful to realize the Heisenberg-Weyl algebra as operators acting in the linear space V of smooth real functions on the configuration space. Then, in Dirac's notations, the pure state is represented by[4]

$$\hat{\rho}=|\psi\rangle\langle\varphi|,\quad\langle\varphi|\psi\rangle=1,\quad|\psi\rangle\in V,\quad\langle\varphi|\in V^*, \tag{25}$$

where the standard inner product is understood. So, the pure state is specified by two real functions on the configuration space. For such states the von Neumann equation is equivalent to two Schrödinger-Zambrini (SZ) equations [60,62],

$$\nu\partial_t|\psi\rangle=\hat{H}|\psi\rangle,\qquad\nu\partial_t\langle\varphi|=-\langle\varphi|\hat{H}. \tag{26}$$

Hereinafter, for simplicity, we restrict ourselves to the case of at most quadratic in momenta Hamiltonians. Besides, we take the metric tensor g_{ij} to be a constant matrix.

After introducing the stochastic phase $\tilde{S}(t,x)$ and the probability density function $\rho(t,x)$ to find a system with the values of extensive parameters x^i,

$$\psi=\rho\exp(-\nu^{-1}\tilde{S}),\qquad\varphi=\exp(\nu^{-1}\tilde{S}), \tag{27}$$

the operators of the total forces $\hat{\mathcal{P}}_\mu=\hat{p}_\mu-A_\mu$ have the averages

$$\langle\hat{\mathcal{P}}_\mu\rangle=\int d^dx\varphi(t,x)[-\nu\partial_\mu-A_\mu(t,x)]\psi(t,x)=\langle\partial_\mu\tilde{S}-A_\mu\rangle,$$

$$\mu=\overline{0,d}, \tag{28}$$

where, for $\mu=0$, we have used the equations of motion (26). Matching thermodynamics with its deformation, we should identify the phase $\tilde{S}$ with the thermodynamic entropy S. Then the SZ equations (26) are invariant with respect to the gauge transformations (10) both with the Hamiltonian (5) and (11).

Consider stochastic deformation of the Hamiltonian dynamical system (5). With the above-mentioned identification, one of the SZ equations (26) is identically satisfied,

$$\nu\partial_t\langle\varphi|=-\langle\varphi|\left[-\partial_tS+\hat{T}_i\upsilon^j(t,\hat{x})+\tfrac{1}{2}\hat{T}_ig^{ij}\hat{T}_j\right], \tag{29}$$

and the other equation becomes the Fokker-Planck equation describing fluctuations of the thermodynamic system,

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[4] Similar projectors also arise when describing projected processes [37].

$$\partial_t \rho = -\partial_i\left(-\frac{\nu}{2} g^{ij}\partial_j \rho + \upsilon^j \rho\right). \tag{30}$$

We see that the coefficients of expansion (5) in terms of T_i are merely the cumulants of the probability distribution of fluctuations.

Deforming the Hamiltonian dynamics generated by Eq. (11), we arrive at two equations: the Fokker-Planck equation (30) and the Hamilton-Jacobi equation (13), with stochastic correction or the Burgers equation [61],

$$A_0 - \partial_t S = \frac{1}{2} g^{ij}(\partial_i S - A_i)(\partial_j S - A_j) + \frac{\nu}{2}\partial_i[g^{ij}(\partial_j S - A_j)], \tag{31}$$

defining the dissipation function $A_0 - \partial_t S$. The form of gauge transformations (10) and the representation (27) show that the gauge group is the Abelian one-dimensional Lie group isomorphic to SO(1, 1). The SZ equations can be rewritten in an explicitly covariant form with respect to the gauge transformations if we group the two functions $\psi(x)$ and $\varphi(x)$ into one vector $\Psi^\alpha(x)$ and define the pseudo-Euclidean scalar product of such vectors as

$$\frac{1}{2}\int d^d x \Psi'^{\alpha}(x)\eta_{\alpha\beta}\Psi^\beta(x) = \frac{1}{2}\int d^d x[\psi'(x),\varphi'(x)]\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} \psi(x) \\ \varphi(x) \end{bmatrix}. \tag{32}$$

Then the SZ equations (26) look like the matrix Schrödinger equation

$$\nu\partial_t \Psi = \begin{bmatrix} \hat{H} & 0 \\ 0 & -\hat{H}^+ \end{bmatrix}\Psi, \tag{33}$$

where the cross denotes a conjugation with respect to the standard inner product. The evolution is generated by the matrix Hamiltonian, which is skew-adjoint with respect to the scalar product (32). On introducing the self-adjoint covariant derivatives

$$\mathcal{P}^\alpha_{\mu\beta} := -\omega^\alpha_\gamma(\nu\partial_\mu\delta^\gamma_\beta + \omega^\gamma_\beta A_\mu), \tag{34}$$

where

$$\omega^\alpha_\beta = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad \omega^2 = 1, \quad \omega^T\eta = -\eta\omega, \tag{35}$$

the SZ equations with the Hamiltonian (11) read

$$-\mathcal{P}_0\Psi = \frac{1}{2}\mathcal{P}_i g^{ij}\mathcal{P}_j\Psi. \tag{36}$$

In this form, the SZ equations are very similar to the quantum-mechanical Schrödinger equation. The difference is that the generator ω of the Lie algebra so(1, 1) appears instead of the generator of $\mathrm{u}(1)\simeq\mathrm{so}(2)$. Further, the equations of motion (36) are immediately generalized to a non-Abelian case. If we have N identical thermodynamic systems in a thermostat, then the global symmetry group for a whole system will be $\mathrm{SO}(N,N)\cap\mathrm{Sp}(N)$. The symplectic group $\mathrm{Sp}(N)$ arises since in the case of N identical systems the matrix $\eta\omega$ is the unit symplectic matrix, which must be preserved by the symmetry transformations. A detailed investigation of peculiarities of non-Abelian systems and their physical interpretation will be given elsewhere. Here we just notice that the group SU(1, 1) locally isomorphic to $\mathrm{SO}(2,2)\cap\mathrm{Sp}(2)/\mathrm{SO}(1,1)$ was studied in the context of generalized coherent states [65–68]. The pair (η,ω) is the analog of an almost generalized product structure on the Whitney sum $TM\oplus T^*M$ (see, for example, [69]).

Let us consider how some standard thermodynamic relations look in our framework. The condition of a detailed balance in the state $|\psi\rangle\langle\varphi|$ becomes

$$\varphi(x)\circ\hat{H}\circ\psi(x) = \psi(x)\circ\hat{H}^+\circ\varphi(x), \tag{37}$$

where $\circ$ means a composition of operators. That is, we can make the gauge transformation so that $\varphi=\psi$, the Hamiltonian $\hat{H}=\hat{H}^+$ having a nonpositive spectrum (see, e.g., [24,37,44]). Then the stochastic phase is identified with a half of the entropy of the whole system (thermostat)+(system). For Hamiltonians of the form (11), with nondegenerate metric g^{ij}, the probability density function $\rho(x)$ in this state is proportional to $\exp[2\nu^{-1}\Sigma(x)]$, where $\Sigma(x) := S(x) - p_i x^i$, provided the Onsager principle (9) is fulfilled. Fixing the extensive variable x^d and applying the WKB method, we obtain that the leading in ν terms of the characteristic function $\ln z(p,x^d)$ of the probability distribution ρ at fixed x^d take the form

$$\ln z(p,x^d) = 2\nu^{-1}\ln Z(p,x^d) + \operatorname{Tr}\ln|\partial^{ij}_p\Phi(p,x^d)|/2 + \cdots . \tag{38}$$

Thus, we arrive at the well-known result that in the leading order the correlators of statistical averages are proportional to the correlators computed with the help of the partition function (1).

In the Heisenberg representation, the operator of the system entropy change is

$$\dot{\hat{S}} = \partial_t\hat{S} + \nu^{-1}[\hat{S},\hat{H}] = \partial_t\hat{S} + \partial_i\hat{S}\frac{\partial\hat{K}}{\partial\hat{p}_i}, \tag{39}$$

where $\partial_i\hat{S}\partial/\partial\hat{p}_i$ is a differentiation of the Heisenberg-Weyl algebra acting on its generators in an obvious manner. Consequently, the gauge invariant entropy production in the whole system (thermostat)+(system) is given by

$$\dot{\hat{\Sigma}} := (\partial_i\hat{S} - \hat{A}_i)\frac{\partial\hat{K}}{\partial\hat{p}_i}, \tag{40}$$

where the dot is just a notation in the case of $F_{ij}\neq 0$. The relation (40) is the stochastic (noncommutative) analog of its thermodynamic counterpart (14). It is reasonable to define the operator of a purely fluctuational entropy production as

$$-\dot{\hat{x}}^i\hat{T}_i = -\nu^{-1}[\hat{x}^i,\hat{H}]\hat{T}_i, \tag{41}$$

which follows from a path-integral representation of its average. This kind of entropy production disappears in the thermodynamic limit. If the system with the Hamiltonian (11) is in the state, where the detailed balance takes place, the average entropy production $\dot{\hat{\Sigma}}$ is zero. The average of the fluctuational term becomes

$$-\nu^{-1}\langle[\hat{x}^i,\hat{K}]\hat{T}_i\rangle = -\nu\langle g^{ij}\partial_{ij}\Sigma\rangle = 2\langle g^{ij}\partial_i\Sigma\partial_j\Sigma\rangle. \tag{42}$$

It is positive and of the order of ν. This is valid in the leading order in ν for any Hamiltonian that allows a detailed balance. Thus the entropy production $\dot{\hat{\Sigma}}$ is caused by equalizing large (macroscopic) differences of intensive parameters of the system and the thermostat, whereas the fluctuational term is responsible for the entropy change made by equalizing small (microscopic) differences of intensive parameters originating from fluctuations. The microscopic deviations can be estimated from the well-known thermodynamic uncertainty relation (see, for example, [10]). In the state with a detailed balance, we have (for a proof see, e.g., [26])

$$\langle(x^i)^2\rangle\langle(\partial_i\Sigma)^2\rangle \geqslant \nu^2/4 \quad \text{(no summation)}. \tag{43}$$

A natural generalization of the above considerations to more realistic nonequilibrium systems possessing spatial gradients of intensive parameters is straightforward. We reduce the system to subsystems of a fixed volume, which are small enough to have homogeneous intensive parameters and sufficiently large to apply a thermodynamic description to them, i.e., the system is in a local thermodynamic equilibrium. Then the simplest model following from first principles of thermodynamics (3) and (8) prescribes a diffusionlike evolution [5,12,32,70],

$$\partial_t\phi^a(t,x) = \int dy g^{ab}(x,y)\left(\frac{\delta S[\phi]}{\delta\phi^b(t,x)} - \frac{\delta S[\phi]}{\delta\phi^b(t,y)}\right),$$

$$g^{ab}(x,y) = g^{ab}(y,x) = g^{ba}(x,y), \tag{44}$$

where $\phi^a(t,x)$ are densities of the extensive variables except the volume, the functional $S[\phi]$ is the thermodynamic entropy of the whole system, and g^{ab} is some positive definite matrix for any x and y, which measures a linear response of the extensive variable a of the subsystem in the point x on a difference of thermodynamic forces b of the subsystems located at x and y. The use of the linear-response relation is justified by small (by construction) deviations of intensive parameters of neighboring subsystems. The total values of extensive variables are conserved by the evolution (44). The Hamilton functional of the form (11) corresponding to Gaussian fluctuations becomes

$$H[t,\phi,\pi] = \frac{1}{4}\int dxdy[\pi_a(x) - \pi_a(y)]g^{ab}(x,y)[\pi_b(x) - \pi_b(y)]$$

$$-A_0[t,\phi], \tag{45}$$

where π_a are the intensive parameters canonically conjugate to ϕ^a. If external thermodynamic force fields are applied, the momenta should be replaced by the covariant derivatives (11). The Hamiltonian formalism is also preferred over the Lagrangian one as the Onsager-Machlup action (7) is nonlocal for local g^{ab}. The functional of a thermodynamic entropy increases with the evolution (44) and acquires a maximum when all the intensive parameters become homogeneous.

Upon stochastic deformation of the model (45), we see that the fluctuating system possesses the states in which the detailed balance (37) takes place,

$$\psi/\varphi \propto \exp\int\lambda_a\phi^a(x)dx, \tag{46}$$

where λ_a are some constants and the stochastic phase $\nu\ln\varphi$ is the thermodynamic entropy. We divide the whole system into a thermostat and the system in it imposing the constraints

$$\langle\varphi|[\pi_a(x) - p_a] = [\pi_a(x) - p_a]|\psi\rangle = 0. \tag{47}$$

Here x runs points of the thermostat and p_a are fixed values of its intensive parameters. These constraints are preserved by the evolution and just say that the intensive variables of the thermostat do not fluctuate. The Hamiltonian corresponding to Eq. (45) is Hermitian and has a nonpositive spectrum. Hence any state of the system satisfying Eq. (47) tends to the ground state described by the probability density functional of the expected form

$$\rho[\phi] \propto \exp\left[2\nu^{-1}\left(S_{\text{sys}}[\phi] - \int_{\text{sys}} dx\, p_a\phi^a(x)\right)\right], \tag{48}$$

where the integral is taken over the system in the thermostat and $S_{\text{sys}}[\phi]$ is the thermodynamic entropy of this system. As before, the average entropy production $\hat{\Sigma}$ relative to this state vanishes. For local g^{ab}, the density of fluctuational entropy production is zero in the thermostat, while it is of the form (42) in the system. As a matter of fact, the matrix $g^{ab}(x,y)$ depends on the fields ϕ^a. A generalization to this case is easily realized along lines [26,36,38].

IV. CONCLUDING REMARKS

Let us mention some possible modifications and generalizations of the formalism evolved here. Notwithstanding we distinguish extensive and intensive parameters, we did not actually use these properties. If the thermodynamic system possesses the "gauge" symmetry

$$x^i\partial_i S = S, \tag{49}$$

i.e., $S(x)$ is a homogeneous function, a division into intensive I and extensive E variables is achieved by

$$\delta I \coloneqq \{x^i T_i, I\} \approx 0, \quad \delta E \coloneqq \{x^i T_i, E\} \approx E. \tag{50}$$

As follows from Eq. (49), the Hessian is degenerate. Therefore, we have to fix the extensive parameter x^d in Eq. (2) and work in the sector of remaining extensive variables and their conjugate. The fixed extensive parameter and its conjugate are expressed in terms of the independent ones by means of Eq. (49). To put it in another way, we fix the "gauge." The division into extensive and intensive variables restricts admissible canonical transformations of the phase space of a thermodynamic system. Such a separation is preserved by arbitrary changes of intensive parameters and only linear transformations (with coefficients depending on the intensive variables) of extensive ones. In geometric terms, we realize the phase space as a Lagrangian fiber bundle [18] with the base parametrized by intensive variables and the fiber represented by the configuration space.

Sometimes it is useful to define an entropy of a thermodynamic system not as the Legendre transform of Φ, but as follows (see, e.g., [40,71]):

$$\tilde{S}(x) = \ln\left[\int dp \exp\left(\sum_{i=1}^{d-1} p_i x^i - \Phi\right)\right], \tag{51}$$

where contours of integration in complex planes are taken so that the integral converges. In a macroscopic limit, this definition coincides with the standard one, which is easy to see using the WKB method. The extensive variables x^i in Eq. (51) are not averaged over the ensemble as in Eq. (2). Rather, they describe one system in it. The intensive variables characterizing this system are taken, by definition, to be $\tilde{p}_i \coloneqq \partial_i \tilde{S}$. They differ slightly from the intensive parameters p_i of the thermostat,

$$\partial_i \tilde{S} = \partial_i S + \frac{1}{2} \partial_{ijk} S \partial_p^{jk} \Phi + \cdots . \tag{52}$$

Assuming the Onsager principle (9) is fulfilled, the system with the Hamiltonian (11) and the entropy (51) decays to the state where a detailed balance takes place. In this state, the characteristic function (38) is strictly proportional to $\ln Z$ up to an irrelevant additive constant.

An entropy of a thermostat is usually described by the term $-p_i x^i$ in the total entropy $\Sigma(x)$, since the intensive parameters of the thermostat are assumed to be nonfluctuating. If such fluctuations become relevant, they can be naturally taken into account in the formalism of stochastic deformation by introducing mixed states. These states are sums of pure states with some weights

$$\hat{\rho} = \sum_p \hat{\rho}_p e^{\sigma(p)}. \tag{53}$$

The function $\sigma(p)$ is proportional to the entropy of the thermostat, while $-p_i x^i$ mentioned above is the entropy of interaction, by analogy with the interaction part of an action functional. The diagonal element of Eq. (53) is proportional to the conditional probability $\rho_p(x) = \varphi(x)\psi_p(x)$, though mixed states are not exhausted by those.

The analogy with mechanics suggests also possible generalizations of a simple Hamiltonian model (11). For example, it is interesting to consider Hamiltonian dynamics on a nonlinear symplectic space describing a thermodynamic system. Passing into the Darboux coordinates, we see that a noncanonical symplectic structure results effectively in a changing of thermodynamic forces and the probability distribution law of fluctuations. Noncanonical symplectic structures appear naturally [37,72] in the case in which small deviations from the Gibbs distribution (1) exist,

$$x^i = \partial_p^i \Phi + \xi^i(p), \tag{54}$$

where ξ^i is a small nongradient vector field. This equality defines a Lagrangian surface of a noncanonical symplectic structure with magnetic fields. For example [72], if the density matrix of the system is proportional to $\exp[-p_i\hat{x}^i - \lambda(p_i\hat{x}^i)^2/2 + O(\lambda^2)]$, where λ is a small parameter, then in the leading orders

$$x^i = \partial_p^i \Phi_0 - \lambda\left[\partial_p^{ij}\Phi_0 p_j - \partial_p^i \Phi_0 \partial_p^j \Phi_0 p_j + \frac{1}{2}\partial_p^{ijk}\Phi_0 p_j p_k \right.$$
$$\left. - \partial_p^{ij}\Phi_0 \partial_p^k \Phi_0 p_j p_k + \partial_p^i \Phi_0 (\partial_p^j \Phi_0 p_j)^2\right] + O(\lambda^2), \tag{55}$$

where $\Phi_0 \coloneqq -\ln Z_0$ with Z_0 taken from Eq. (1). The last term in the brackets is nongradient. Defining a thermodynamic entropy as the Legendre transform of the Massieu function Φ_0, we arrive at the first law of thermodynamics with magnetic fields. The gradient part can be absorbed into the entropy by a gauge transformation. Another evident generalization of the model (11) consists in introducing non-Abelian gauge fields. We only touched on the problem in Sec. III and formulated the "matter" dynamics. The next step is to introduce the action functional for the gauge fields. The gauge symmetries of gauge fields' action seem to be spontaneously broken, though a form of the action and a mechanism of the symmetry breaking are the subjects for further research.

Besides, we saw that quantum and stochastic mechanics differ from each other by a symmetry group only. Namely, the Heisenberg-Weyl algebra is a Lie algebra with commutation relations

$$[e_1, e_2] = e_3, \quad [e_1, e_3] = [e_2, e_3] = 0, \tag{56}$$

where e_1, e_2, and e_3 are its generators and, for brevity, we consider a two-dimensional phase space. This algebra includes an Abelian ideal spanned on e_3. A general form of the Lie group corresponding to this ideal is $\mathrm{U}^n(1) \times \mathrm{SO}^k(1,1)$. In the two simplest cases $n=1$, $k=0$ and $n=0$, $k=1$, we obtain quantum and stochastic mechanics, respectively. So, one can speculate about their unification by introducing a larger group containing the subgroups U(1) and SO(1,1).

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