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Weak invariants in dissipative systems: action principle and Noether charge for kinetic theory

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In non-equilibrium classical thermostatistics, the state of a system may be described by not only dynamical/thermodynamical variables but also a kinetic distribution function. This 'double structure' bears some analogy with that in quantum thermodynamics, where both dynamical variables and the Hilbert space are involved. Recently, the concept of weak invariants has repeatedly been discussed in the context of quantum thermodynamics. A weak invariant is defined in such a way that its value changes in time but its expectation value is conserved under time evolution prescribed by a kinetic equation. Here, a new aspect of a weak invariant is revealed for the classical Fokker–Planck equation as an example of classical kinetic equations. The auxiliary field formalism is applied to the construction of the action for the kinetic equation. Then, it is shown that the auxiliary field is a weak invariant and is the Noether charge. The action is invariant under the transformation generated by the weak invariant. The result may shed light on possible roles of the symmetry principle in the kinetic descriptions of non-equilibrium systems.

This article is part of the theme issue 'Fundamental aspects of nonequilibrium thermodynamics'.

1. Introduction

Quantum thermodynamics [1–3] is of importance for its possible contributions to classical thermodynamics in the non-equilibrium regime, in addition to its relevance to e.g. nanoscience and quantum information. A point is the fact that an element of a classical system is fundamentally described by a set of dynamical/thermodynamical variables, whereas in quantum mechanics the Hilbert space also accompanies. This 'double structure' in quantum thermodynamics leads to diversity of the bath concepts. A typical example is the dephasing bath [4], the role of which is to realize decoherence of a quantum state and therefore has no classical counterparts. As long as limited to classical equilibrium thermodynamics concerns, the bath simply implies the heat bath. In non-equilibrium classical thermodynamics, however, a situation becomes somewhat analogous to quantum thermodynamics if the kinetic approach is employed, where both dynamical/thermodynamical variables and time evolution of a probability distribution function of a system under consideration have to be treated.

Thermodynamic processes of interest are usually characterized by conserved values of quantities and variables. Examples are the isothermal, isochoric, isobaric and isoentropic processes. In a couple of recent works [5,6] on finite-time quantum thermodynamics, a process termed the isoenergetic process has been studied by the use of the Lindblad equation [7,8]. Along such a process, the internal energy is kept constant. This requires the concept of the energy bath with no counterparts in equilibrium classical thermodynamics and may be realized by the energy transfer technique [9,10]. Such an exotic process manifests the implications of the quantum mechanical violation of the law of equipartition of energy to thermodynamics since it is different from the isothermal process. There, although the Hamiltonian of an objective subsystem explicitly depends on time and therefore its spectrum is not constant in time, the internal energy, i.e. its expectation value, remains constant. This condition turns out to be able to determine the Lindbladian operators without recourse to detailed knowledge about an interaction between the subsystem and the energy bath [5,6].

In general, a time-dependent observable is referred to as a weak invariant [11] if its spectrum depends on time but the expectation value is conserved in the course of time evolution described by a master equation such as the Lindblad equation. The time-dependent Hamiltonians in the isoenergetic processes discussed in [5,6] are thus weak invariants. By contrast, a time-dependent observable with the time-independent spectrum is to be called a strong invariant. The Lewis–Riesenfeld invariant [12] associated with a time-dependent Hamiltonian is an example of strong invariants. It has been applied to a wide variety of problems including quantum optics and related systems [13–15], non-stationary quantum field theory [16–18], geometric phases [19–21] quantum computation [22] and quantum cosmology [23]. It is worth emphasizing that the classical counterpart of the Lewis–Riesenfeld strong invariant can be derived by Noether's theorem [24] (see also [25] for a simplified discussion). Its generalization to dissipative systems has recently been presented in [11], where the weak invariant of the time-dependent quantum damped oscillator has explicitly been constructed by the use of the Lindblad equation.

The action principle for kinetic theory has repeatedly been discussed in the literature. Among others, the approach [26,27] should be noticed, in particular. There, an auxiliary field is introduced in order for the construction of the action functional for the Liouville–von Neumann equation, and thus this approach is referred to as the auxiliary field formalism. A primary reason for the introduction of such an extra field is due to the fact that the Liouville–von Neumann equation is a first-order differential equation in time for a density matrix. Although the Liouville–von Neumann equation possesses time-reversal invariance (for autonomous isolated systems), more general master equations may violate such symmetry. For example, the Lindblad equation repeatedly mentioned above describes dissipative dynamics. Then, the auxiliary field formalism comes to play a prominent role: the action can be constructed for dissipative kinetics through the extension of the space of variables. It is also mentioned that this formalism offers a powerful tool for obtaining approximate solutions in analytic forms if combined with the Rayleigh–Ritz method [27,28].

Recently, the auxiliary field formalism has been applied to classical fractional kinetic equations [28,29] as well as a general quantum master equation [30]. It has been found that the auxiliary field introduced in the action may actually be a weak invariant of the corresponding master equation. This fact indicates the existence of a certain deeper structure that must be related to the symmetry principle behind kinetic theory. Understanding such a principle may, in turn, cast fresh light on non-equilibrium thermodynamics even at the classical level.

In this paper, the action principle and weak invariants are studied in the context of classical kinetic theory. Although a specific form of a kinetic equation is not needed as long as it is linear, the Fokker–Planck equation [31,32] is employed as an important example for the sake of clarity. The Fokker–Planck equation is derived from the Langevin equation that describes the irreversible relaxation processes [33], and therefore it is of direct relevance to non-equilibrium thermodynamics. In addition, the weak invariant of the Fokker–Planck equation has already been discussed in [34]. Now, the primary purpose of the present work is to show how the auxiliary field as the weak invariant in the action principle plays a role of the Noether charge and accordingly the action I satisfies

$$\Delta_\varepsilon I = 0, \tag{1.1}$$

where Δ_ε stands for the infinitesimal transformation generated by the weak invariant. This result may give new insight into possible roles of the symmetry principle in kinetic theory of dissipative systems and associated non-equilibrium thermodynamic processes.

The present paper is organized as follows. In §2, the concept of weak invariants is explained for the Fokker–Planck equation, and the action principle for the equation is formulated by the use of the auxiliary field. Then, the auxiliary field is shown to be a weak invariant. In §3, the canonical formulation is developed, and the action is shown to be invariant under the transformation generated by the auxiliary field as a weak invariant. Thus, the weak invariant is found to be the Noether charge. Section 4 is devoted to concluding remarks.

2. Weak invariant and action principle for Fokker–Planck equation

Consider the Fokker–Planck equation of the following form [31,32]:

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x}[K(x,t)P(x,t)] + \frac{\partial^2}{\partial x^2}[D(x,t)P(x,t)]$$

$$\equiv L_t[P(x,t)]. \tag{2.1}$$

Here, $P(x,t)\,dx$ is the probability of finding the value of a physical variable x in the interval $[x, x+dx]$ at time t. The domain of the probability distribution function is taken to be $(-\infty,\infty) \times [t_i, t_f]$. The operator L_t is allowed to possess time dependence through K in the drift term and the positive diffusion coefficient D. Generalization to the case of many variables is straightforward. Equation (2.1) does not possess time-reversal invariance, in general. The quantity conserved under time evolution is nothing but the total probability $\int_{-\infty}^{\infty} dx P(x,t)$ that may be set equal to unity.

A quantity, $J(x,t)$, is said to be a weak invariant associated with equation (2.1) if it satisfies

$$\frac{\partial J(x,t)}{\partial t} + L_t^{\dagger}[J(x,t)] = 0, \tag{2.2}$$

where $L_t^{\dagger} \equiv K(x,t)\partial/\partial x + D(x,t)\partial^2/\partial x^2$ is the adjoint of L_t in equation (2.1). Then, it can immediately be ascertained that the expectation value $\langle J \rangle = \int_{-\infty}^{\infty} dx J(x,t)P(x,t)$ is conserved:

$$\frac{d\langle J \rangle}{dt} = 0. \tag{2.3}$$

Here, the probability distribution function and its spatial derivative need be required to decrease at the spatial infinities sufficiently rapidly. On the other hand, a weak invariant can be free from boundary conditions as long as its expectation value is finite and equation (2.3) holds. Accordingly, there exist large degrees of freedom in its choice. This is certainly an advantageous

point since it implies that a wide class of quantities satisfying equation (2.2) can be chosen as a weak invariant, depending on physical interest. However, as seen in the subsequent discussion, a weak invariant is subject to the final condition, not the initial condition.

Although the first moment of the weak invariant satisfies equation (2.3), the higher moments do not, in general. In fact, the variance $(\Delta J)^2 = \langle J^2 \rangle - \langle J \rangle^2$ monotonically increases as follows:

$$\frac{\mathrm{d}(\Delta J)^2}{\mathrm{d}t} = 2\langle D(J')^2 \rangle, \tag{2.4}$$

where $J' \equiv \partial J(x, t)/\partial x$.

Because of its irreversible nature and the structure of the first-order time derivative, it is non-trivial to develop the action principle for the Fokker–Planck equation. A quantum mechanical analogue of this issue has been studied in [26,27]. There, an auxiliary field Λ has been introduced for the extension of the space of variables, by which the action can be constructed. In the present case, the action for equation (2.1) reads

$$I[P, \Lambda] = \int_{t_i}^{t_f} \mathrm{d}t \int_{-\infty}^{\infty} \mathrm{d}x \, £ - \frac{1}{2} \int_{-\infty}^{\infty} \mathrm{d}x (\Lambda P|_{t=t_i} + \Lambda P|_{t=t_f}), \tag{2.5}$$

where $£$ is the Lagrangian density given by

$$£ = \frac{1}{2} \left(\Lambda \frac{\partial P}{\partial t} - \frac{\partial \Lambda}{\partial t} P \right) - \Lambda \left(-\frac{\partial}{\partial x}(KP) + \frac{\partial^2}{\partial x^2}(DP) \right). \tag{2.6}$$

The second term on the right-hand side in equation (2.5) is the temporal boundary one that is peculiar in the auxiliary field formalism [26,27]. Upon taking the variation of the action, one should take into account that $P(x, t)$ is a probability distribution function satisfying the normalization condition, which needs be treated as a constraint. However, it is actually not necessary to add such a constraint to the action, since it can be eliminated by the redefinition of the auxiliary field $\Lambda(x, t)$. Indeed, if the auxiliary field is redefined as

$$\Lambda(x, t) \to \Lambda(x, t) + \int_{t}^{t_f} \mathrm{d}s \, \lambda(s), \tag{2.7}$$

then, the term

$$\int_{t_i}^{t_f} \mathrm{d}t \lambda(t) \left(\int_{-\infty}^{\infty} \mathrm{d}x P(x, t) - \int_{-\infty}^{\infty} \mathrm{d}x P(x, t_i) \right), \tag{2.8}$$

automatically appears in the action. This is nothing but the constraint on the normalization condition, if the initial probability distribution function is normalized. And, $\lambda(t)$ plays a role of the Lagrange multiplier. It is noted that equation (2.7) does not change the final condition $\Lambda(x, t_f)$.

The variations of the action in equation (2.5) with respect to $\Lambda(x, t)$ and $P(x, t)$ yield

$$\delta_\Lambda I[P, \Lambda] = \int_{t_i}^{t_f} \mathrm{d}t \int_{-\infty}^{\infty} \mathrm{d}x \left(\frac{\partial P}{\partial t} + \frac{\partial}{\partial x}(KP) - \frac{\partial^2}{\partial x^2}(DP) \right) \delta \Lambda - \int_{-\infty}^{\infty} \mathrm{d}x P \delta \Lambda|_{t=t_f} \tag{2.9}$$

and

$$\delta_P I[P, \Lambda] = -\int_{t_i}^{t_f} \mathrm{d}t \int_{-\infty}^{\infty} \mathrm{d}x \left(\frac{\partial \Lambda}{\partial t} + K \frac{\partial \Lambda}{\partial x} + D \frac{\partial^2 \Lambda}{\partial x^2} \right) \delta P - \int_{-\infty}^{\infty} \mathrm{d}x \Lambda \delta P|_{t=t_i}, \tag{2.10}$$

respectively.

From equation (2.9), the Fokker–Planck equation (2.1) is derived if the final condition $\delta \Lambda(x, t_f) = 0$ is imposed, i.e. the final condition on the auxiliary field being fixed. In this respect, recall also that equation (2.7) keeps $\Lambda(x, t_f)$ unchanged.

On the other hand, the equation for the auxiliary field

$$\frac{\partial \Lambda(x,t)}{\partial t} + L_t^{\dagger}[\Lambda(x,t)] = 0, \tag{2.11}$$

is obtained from equation (2.10) under the initial condition $\delta P(x, t_i) = 0$, i.e. $P(x, t_i)$ being fixed. This equation shows that the spatial integral of the auxiliary field is not necessarily a conserved quantity, in contrast with the probability distribution function.

A crucial point is the fact that equations (2.2) and (2.11) are identical to each other. It is therefore concluded that *the auxiliary field introduced into the action for the Fokker–Planck equation is a weak invariant associated with the equation*. In this way, the auxiliary field, which used to be a mathematical object introduced rather formally, is now endowed with a physical significance.

3. Weak invariant as Noether charge

Canonical theory is constructed from the Lagrangian density in equation (2.6). The canonical momentum densities conjugate to the probability distribution function and auxiliary field are $\Pi_P = \partial \pounds / \partial (\partial P / \partial t) = \Lambda / 2$ and $\Pi_\Lambda = \partial \pounds / \partial (\partial \Lambda / \partial t) = -P/2$, respectively. $\partial P / \partial t$ and $\partial \Lambda / \partial t$ cannot be solved in terms of the canonical momentum densities. Accordingly, the following constraints are present: $\chi_1 \equiv \Pi_P - \Lambda / 2 \approx 0$, $\chi_2 \equiv \Pi_\Lambda + P/2 \approx 0$, where the symbol '$\approx$' stands for the weak equality in Dirac's notation [35]. The equal-time Poisson bracket is defined in terms of the functional derivatives as follows: $\{A(t), B(t)\} = \int_{-\infty}^{\infty} dx \sum_{i=1,2} (\delta A(t)/\delta Q_i(x,t) \cdot \delta B(t)/\delta \Pi_i(x,t) - \delta A(t)/\delta \Pi_i(x,t) \cdot \delta B(t)/\delta Q_i(x,t))$. In this expression, $Q_1(x,t)$, $Q_2(x,t)$, $\Pi_1(x,t)$ and $\Pi_2(x,t)$ denote $P(x,t)$, $\Lambda(x,t)$, $\Pi_P(x,t)$ and $\Pi_\Lambda(x,t)$, respectively. In general, $A(t)$ and $B(t)$ are functionals that are the spatial integrals of functions of these four fields. Then, the basic equal-time Poisson bracket relations are $\{P(x,t), \Pi_P(x',t)\} = \delta(x - x')$, $\{\Lambda(x,t), \Pi_\Lambda(x',t)\} = \delta(x - x')$, and all the other combinations vanish. Therefore, it follows that $\{\chi_i(x,t), \chi_j(x',t)\} = -\varepsilon_{ij} \delta(x - x')$, where ε_{ij} is the Levi–Civita symbol in two dimensions (i.e. $\varepsilon_{12} = -\varepsilon_{21} = 1$, $\varepsilon_{11} = \varepsilon_{22} = 0$). So, the constraints are of the second class [35]. A standard way of eliminating them is to use the Dirac bracket: $\{A(t), B(t)\}_D = \{A(t), B(t)\} - \sum_{i,j=1,2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dy dy' \{A(t), \chi_i(y,t)\} C_{ij}(y,y') \{\chi_j(y',t), B(t)\}$, where $C_{ij}(y,y')$ is the quantity satisfying $\sum_{k=1,2} \int_{-\infty}^{\infty} dy \{\chi_i(x,t), \chi_k(y,t)\} C_{kj}(y,y') = \delta_{ij} \delta(x - y')$ and is found to be $C_{ij}(y,y') = \varepsilon_{ij} \delta(y - y')$. The second-class constraints become the identical equalities in this formalism. Then, the basic equal-time Dirac bracket relations are given as follows:

$$\{P(x,t), \Lambda(x',t)\}_D = \delta(x - x'), \quad \{P(x,t), P(x',t)\}_D = 0 \quad \{\Lambda(x,t), \Lambda(x',t)\}_D = 0. \tag{3.1}$$

The first relation implies that the probability distribution function and auxiliary field are canonically conjugate to each other. It should be noted that the first relation never contradicts the normalization condition on the probability distribution function since such a condition is, as mentioned after equation (2.6), a constraint (i.e. a weak equation): $\int_{-\infty}^{\infty} dx P(x,t) \approx \int_{-\infty}^{\infty} dx P(x, t_i)$.

The Hamiltonian density is given by the Legendre transformation of the Lagrangian density in equation (2.6). Its spatial integration is the Hamiltonian and is explicitly given by $H(t) = \int_{-\infty}^{\infty} dx \Lambda(x,t) L_t[P(x,t)] = \int_{-\infty}^{\infty} dx L_t^{\dagger}[\Lambda(x,t)] P(x,t)$. Then, equations (2.1) and (2.11) are rewritten as $\partial P(x,t)/\partial t = \{P(x,t), H(t)\}_D$ and $\partial \Lambda(x,t)/\partial t = \{\Lambda(x,t), H(t)\}_D$, respectively. Thus, the Fokker–Planck equation is recast in the Liouvillian form.

The primary purpose of the present work is to show that the action is invariant under the transformation generated by the weak invariant. For this, it is convenient to set up the non-equal-time Dirac bracket relations. Such relations are obtained as follows. Solve equations (2.1) and (2.11) formally as

$$P(x,t) = T \exp \left(\int_{t'}^{t} ds L_s \right) P(x,t') \tag{3.2}$$

and

$$\Lambda(x,t') = T \exp \left(-\int_{t}^{t'} ds L_s^{\dagger} \right) \Lambda(x,t), \tag{3.3}$$

respectively, where T stands for the chronological symbol responsible for ordering of the product of operators non-commutative at different times [36]. From these, the relations in equation (3.1) are generalized as follows:

$$\{P(x,t), \Lambda(x',t')\}_D = T \exp\left(-\int_t^{t'} ds L_s'^\dagger\right) \delta(x-x'), \quad \{P(x,t), P(x',t')\}_D = 0$$
$$\{\Lambda(x,t), \Lambda(x',t')\}_D = 0, \tag{3.4}$$

where $L_t'^\dagger$ denotes $L_t^\dagger$ in equation (2.2) with respect to the variable x'.

Now, the invariant nature of the action can be made manifest. The transformation of a certain physical quantity, say Q, generated by the weak invariant Λ is defined by

$$\Delta_\varepsilon Q = \{Q, G_\varepsilon\}_D, \tag{3.5}$$

where

$$G_\varepsilon \equiv \int_{-\infty}^{\infty} dx\, \varepsilon(x,t)\Lambda(x,t), \tag{3.6}$$

with $\varepsilon(x,t)$ being an arbitrary infinitesimal function on a compact support so that the integral in equation (3.6) converges. Then, taking the action in equation (2.5) as Q, one finds

$$\Delta_\varepsilon I = \{I, G_\varepsilon\}_D$$
$$= -\int_{t_i}^{t_f} dt \int_{-\infty}^{\infty} dx \left(\frac{\partial \Lambda(x,t)}{\partial t} + L_t^\dagger[\Lambda(x,t)]\right) \times \int_{-\infty}^{\infty} dx'\, \varepsilon(x',t') T \exp\left(-\int_t^{t'} ds L_s'^\dagger\right) \delta(x-x')$$
$$- \int_{-\infty}^{\infty} dx\, \Lambda(x,t_i)\Delta_\varepsilon P(x,t_i). \tag{3.7}$$

Since the initial probability distribution function is fixed, the last term vanishes. Therefore, from equation (2.11), it follows that equation (1.1) in fact holds. Consequently, the action is seen to be invariant under the transformation generated by the weak invariant. This result offers a reinterpretation of the variation in equation (2.10) in terms of the symmetry principle.

4. Concluding remarks

The action principle has been studied for the Fokker–Planck equation, and the associated weak invariant has been shown to be the Noether charge generating the transformation, under which the action remains unchanged.

It is noted that the variational approach discussed in the present work is radically different from the one that is directly applied to thermodynamic variables and is somewhat criticized in [37].

The theory developed here is free from a specific form of a kinetic equation (at least, as long as it is linear). For example, it is straightforward to apply it to fractional kinetics with spatio-temporal non-locality. In fact, the action principle for the fractional Fokker–Planck equation and the corresponding canonical theory have already been constructed [29].

It is also pointed out that there have been continuous research activities of non-local non-equilibrium thermodynamics [38–41]. It may be of interest to examine such discussions from the viewpoint of generalized kinetics as in the traditional shift from the kinetic stage to the hydrodynamic one. Weak invariants and their possible roles in generalized kinetics are yet to be explored.

As long as limited to genuine classical thermodynamics, the bath implies the heat bath even in the non-equilibrium regime, and accordingly exotic baths such as the energy bath mentioned in §1 do not exist there. However, the thermodynamic formalism has high-level universality. Thermodynamic analogues are ubiquitously observed in various fields such as econophysics, physics of seismicity or time series analysis, in general. Non traditional approaches including the present are expected to widen the realm of the thermodynamic formalism.

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