Renormalization of transport equations in Fokker-Planck models

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This paper is concerned with the derivation of nonlinear fluctuation-renormalized transport equations of a fluctuating thermodynamic system, on the assumption that the macroscopic variables defining a state undergo a Fokker-Planck process. It is shown that the renormalization effect may consist of two parts: a renormalization of the thermodynamic forces and a renormalization of the transport coefficients. Closed analytical expressions for the renormalized quantities in terms of the bare quantities appearing in the Fokker-Planck equation are derived. A scheme for the approximate evaluation of these expressions is given.

I. INTRODUCTION

In the study of many problems in nonequilibrium statistical thermodynamics one is led to a complete set of macroscopic variables which undergo a continuous Markovian process.[1] The master equation of such a stochastic process is the Fokker-Planck equation. The quantities which one would like to determine are certain ensemble-averaged properties, the most simple of which are the mean values of the macroscopic variables. In most problems which are currently receiving attention the Fokker-Planck equation is nonlinear. Owing to this nonlinearity the mean values are coupled to the fluctuations of the macroscopic variables. This complicates the derivation of the transport equations describing the mean relaxation of an ensemble. The need for a fluctuation renormalization of the transport equations has been pointed out by Zwanzig,[2] and several renormalization strategies have been proposed by Nordholm and Zwanzig.[3] They determine the higher-order cumulants which couple to the mean values using a straightforward generalization of Picard's method of successive approximations. Although systematic, such an expansion is not adequate if one is interested in the long-time limit. Being aware of this, Nordholm and Zwanzig modify the procedure and propose some zeroth-order approximations which are particularly reasonable in the long-time limit. However, in order to obtain higher-order corrections, they must return to the approximate solutions of the equations of motions of the cumulants obtained by Picard's method.

Another means of treating fluctuation renormalization has been put forward by Mori and Fujisaka.[4] They used a projection operator which extracts the linear part of the fluctuation-renormalized transport equations. Their equations give a correct description of the long-time behavior when the system is already in the vicinity of the equilibrium state. However, the method does not allow one to determine corrections which are important if the initial state is not near equilibrium. In the present paper, we analyze the problem in a more complete way and derive nonlinear fluctuation-renormalized transport equations which are practically useful in the short-time limit as well as in the long-time limit, thus combining the advantages of the previous methods.

The paper is organized as follows: In Sec. II we present the type of Fokker-Planck models which we are considering. The Fokker-Planck equation is nonlinear because the stationary distribution may be non-Gaussian and the bare transport coefficients may depend on the state of the system. We show how the problem of fluctuation renormalization arises.

The renormalization procedure can be split into two parts. The thermodynamic forces which cause the fluxes are renormalized if the stationary distribution is non-Gaussian. This step is discussed in Sec. III. The second renormalization step leads to a renormalization of the transport coefficients. In Sec. IV we obtain exact expressions for the renormalized transport coefficient using time-dependent projection-operator techniques. These techniques have been used widely in connection with the Liouville equation.[5] We propose a similar approach in connection with the Fokker-Planck equation.

For practical purposes the exact expressions which contain nonlinearities of all orders must be approximated. A systematic approximation scheme which is appropriate whenever the static distribution is Gaussian in the vicinity of its maximum is given in Sec. 5. The approximation is in terms of the same small parameter needed to obtain the Fokker-Planck approximation from the underlying statistical mechanics.[6]

II. FOKKER-PLANCK MODEL

We consider a system whose macroscopic state is described by a set $a=(a^1, \ldots, a^i, \ldots, a^n)$ of macroscopic variables forming the state space Σ.

In a stochastic theory which includes the fluctuations of the variables a we ask for the probability $p(a,t)da$ to find the system at time t in the volume element da around the state a. We assume that the time evolution of this probability is governed by a Fokker-Planck equation of the form[6]

$$\frac{\partial}{\partial t} p(a,t) = \frac{\partial}{\partial a^i} k_B L^{ij}(a)\left(\frac{\partial p(a,t)}{\partial a^j} - \frac{p(a,t)}{w(a)}\frac{\partial w(a)}{\partial a^j}\right), \tag{2.1}$$

where a summation must be carried out over the repeated indices; k_B denotes Boltzmann's constant, which has been introduced in order that the "bare transport coefficients" L^{ij} have the usual units of phenomenological thermodynamics, $w(a)$ is the stationary solution of the Fokker-Planck equation. For a closed system, $w(a)$ is of the form

$$w(a) \propto e^{(1/k_B)S(a)}, \tag{2.2}$$

where $S(a)$ is the (bare) entropy. If the system interacts with an environment, $S(a)$ must be replaced by the adequate potential. This change, however, is purely formal.

The Fokker-Planck equation (2.1) may also be written in the more familiar form

$$\frac{\partial}{\partial t} p(a,t) = \frac{\partial}{\partial a^i}\left(-K^i(a) + k_B \frac{\partial}{\partial a^j} D^{ij}(a)\right) p(a,t), \tag{2.3}$$

with the Fokker-Planck drift

$$K^i = \frac{1}{w}\frac{\partial}{\partial a^j} k_B L^{ij} w = L^{ij}\frac{\partial S}{\partial a^j} + k_B \frac{\partial L^{ij}}{\partial a^j}, \tag{2.4}$$

and the diffusion matrix

$$D^{ij} = \tfrac{1}{2}(L^{ij} + L^{ji}), \tag{2.5}$$

which is assumed to be positive.

In the following, the Boltzmann constant k_B will also be used as a small parameter. In some systems the transport coefficients are inversely proportional to the system size,[7] so that an expansion in terms of k_B is equivalent to an expansion in terms of the inverse system size. A similar connection of k_B with a small parameter is typical for many Fokker-Planck models, because an equation of the form (2.3) can be obtained from more basic equations within a statistical-mechanical theory[8] only if such a small parameter exists.

The mean values $\bar{a}$ of the state variables a are given by

$$\bar{a}^i(t) = \mathrm{tr}[p(a,t)a^i], \tag{2.6}$$

where tr denotes integration over the entire state space Σ. By means of (2.3) we obtain for the time rates of change of the mean values

$$\frac{d}{dt}\bar{a}^i(t) = \mathrm{tr}[p(a,t)K^i(a)]. \tag{2.7}$$

If the distribution $p(a,t)$ is sharply peaked about the mean $\bar{a}(t)$ we have

$$\mathrm{tr}[p(a,t)K^i(a)] \simeq K^i(\bar{a}(t)). \tag{2.8}$$

This is, however, often too crude an approximation. The fluctuations of the variables a lead to corrections to (2.8). A systematic way to determine those corrections is the aim of this work.

The broadening of an initially sharp distribution is caused by the diffusion term $k_B(\partial^2/\partial a^i \partial a^j)D^{ij}p$ of the Fokker-Planck equation (2.3). Since this term is proportional to k_B the distribution remains sharp for $k_B \to 0$. From (2.4) and (2.7) we find in the limit $k_B \to 0$

$$\frac{d}{dt}\bar{a}^i(t) = L^{ij}(\bar{a}(t))\,\lambda_j(\bar{a}(t)), \tag{2.9}$$

where we have introduced the "bare thermodynamic forces"

$$\lambda_i(a) = \frac{\partial S(a)}{\partial a^i}. \tag{2.10}$$

Equations (2.9) are the deterministic equations of motion.[6] We refer to them also as the "bare transport equations." They are exact for a linear system, where the transport coefficients L^{ij} are constant and where the entropy $S(a)$ is a quadratic function of the variables a. Then, $K^i(a)$ and $\lambda_i(a)$ are linear functions of a and (2.9) follows from (2.4) and (2.7) without further assumption.

In a nonlinear system, Eqs. (2.9) provide only a lowest-order approximation to the correct "renormalized transport equations." The nonlinearity may have two origins. First, the stationary distribution $w(a)$ may be non-Gaussian, so that the thermodynamic forces $\lambda_i(a)$ are nonlinear functions of a. Second, the transport coefficients L^{ij} may depend on the state a. The first kind of nonlinearity shows up in the statics of the system, while the second is purely dynamical.

III. RELEVANT DISTRIBUTION AND RENORMALIZED THERMODYNAMIC FORCES

There is a well-known evolution criterion[6,9] associated with the Fokker-Planck equation (2.1). Let us define a functional $H(p(a,t))$ of the distribution $p(a,t)$ by

$$H(p(a,t)) = -k_B\,\mathrm{tr}[p(a,t)\ln p(a,t)/w(a)]. \tag{3.1}$$

By means of the Fokker-Planck equation (2.1) and Eq. (2.5) we find for the time rate of change[6,9] of $H(p)$

$$\frac{\partial}{\partial t} H(p(a,t)) = k_B^2 \,\mathrm{tr}\left(p(a,t) D^{ij}(a) \frac{\partial \sigma(a,t)}{\partial a^i} \frac{\partial \sigma(a,t)}{\partial a^j}\right) \geq 0\,, \quad (3.2)$$

where

$$\sigma(a,t) = \ln p(a,t)/w(a)\,. \quad (3.3)$$

Hence $H(p)$ increases in time it reaches its maximum for the stationary state $w(a)$ which is approached as $t \to \infty$.

Assume that we know the mean values $\bar{a}(t)$ of the macroscopic variables; we wish to know the distribution $p(a,t)$. Since we cannot determine $p(a,t)$ completely, we will look for a "relevant distribution" $\bar{p}(a,t)$ which is an optimal choice of $p(a,t)$ corresponding to the information given. It is natural to determine $\bar{p}(a,t)$ by the requirement that it maximize $H(p(a,t))$ under the constraints

$$\mathrm{tr}\,\bar{p}(a,t) = 1 \quad (3.4)$$

and

$$\mathrm{tr}[\bar{p}(a,t)a^i] = \bar{a}^i(t)\,. \quad (3.5)$$

By standard variational techniques we find that $\bar{p}(a,t)$ is of the form

$$\bar{p}(a,t) = Z^{-1}(t) w(a) e^{-(1/k_B)\bar{\lambda}_i(t) a^i}\,, \quad (3.6)$$

where

$$Z(t) = \mathrm{tr}[w(a) e^{-(1/k_B)\bar{\lambda}_i(t) a^i}]\,. \quad (3.7)$$

The parameters $\bar{\lambda}(t)$ are determined by (3.5) as functions of the mean values $\bar{a}(t)$. Consequently, $\bar{p}(a,t)$ is also a function of the $\bar{a}(t)$ and has no explicit time dependence: $\bar{p}(a,t) = \bar{p}(a,\bar{a}(t))$. With (2.2) we see that (3.6) may be written

$$\bar{p}(a,t) \propto e^{(1/k_B)[S(a) - \bar{\lambda}_i(t) a^i]}\,. \quad (3.8)$$

This distribution is of the form of the stationary distribution of the system in the presence of external forces that displace it from equilibrium.[9] It is natural to split the precise distribution $p(a,t)$ into

$$p(a,t) = \bar{p}(a,t) + \delta p(a,t)\,, \quad (3.9)$$

where $\bar{p}(a,t)$ is already determined by the mean values and describes a stationary system constrained to these mean values, while $\delta p(a,t)$ describes the dynamical corrections typical for a transient state $p(a,t)$.

Besides the "bare entropy" $S(a)$, which is a function of the actual values of the macroscopic variables a, we introduce a "renormalized entropy" $\bar{S}(\bar{a})$ as a function of the mean values $\bar{a}$ by

$$\bar{S}(\bar{a}(t)) = -k_B \,\mathrm{tr}[\bar{p}(a,t) \ln \bar{p}(a,t)/w(a)]\,; \quad (3.10)$$

$\bar{S}(\bar{a}(t))$ is just the maximal value of the functional $H(p)$ under the constraints (3.4), (3.5). Using Eqs. (3.5)–(3.7) we find

$$\bar{S}(\bar{a}) = k_B \ln Z + \bar{\lambda}_i \bar{a}^i\,, \quad (3.11)$$

and further

$$\bar{a}^i = -\frac{\partial k_B \ln Z}{\partial \bar{\lambda}_i}\,, \quad (3.12)$$

as well as

$$\bar{\lambda}_i = \frac{\partial \bar{S}}{\partial \bar{a}^i}\,. \quad (3.13)$$

The $\bar{\lambda}$ are derived from the renormalized entropy $\bar{S}(\bar{a})$ in the same way as the bare thermodynamic forces λ are derived from $S(a)$. We call the parameters $\bar{\lambda}$ "renormalized thermodynamic forces." The renormalization of the thermodynamic forces is due to the non-Gaussian behavior of the fluctuations in the stationary state. If the statics is Gaussian, the $\bar{\lambda}$ coincide with the bare thermodynamic forces λ.

From (3.6) and (3.7) we find

$$\frac{\partial \bar{p}(a,t)}{\partial \bar{\lambda}_i(t)} = -\frac{1}{k_B} \bar{p}(a,t)[a^i - \bar{a}^i(t)]\,, \quad (3.14)$$

which yields with (3.5)

$$\frac{\partial \bar{a}^i(t)}{\partial \bar{\lambda}_j(t)} = -\frac{1}{k_B} \bar{\sigma}^{ij}(t)\,, \quad (3.15)$$

where

$$\bar{\sigma}^{ij}(t) = \mathrm{tr}[\bar{p}(a,t) a^i a^j] - \bar{a}^i(t) \bar{a}^j(t) \quad (3.16)$$

is the variance matrix of the macroscopic variables in the state $\bar{p}(a,t)$. Since $\bar{\sigma}^{ij}(t)$ is a positive definite matrix so is its inverse, and we see with (3.13) and (3.15) that

$$\frac{\partial^2 \bar{S}}{\partial \bar{a}^i \partial \bar{a}^j} = -k_B [\bar{\sigma}^{ij}(t)]^{-1} \quad (3.17)$$

is negative definite, which means that the renormalized entropy $\bar{S}(\bar{a})$ is a convex function of the variables $\bar{a}$. This property, which is generally required for the thermodynamic entropy[10] may not hold for the bare entropy $S(a)$.

IV. DERIVATION OF RENORMALIZED TRANSPORT EQUATIONS

Assume that we apply constant external forces to the system and wait until it reaches the stationary state in the presence of these forces. Then the state of the system is of the form

$$p(a,0) \propto e^{(1/k_B)[S(a) - \bar{\lambda}_i(0) a^i]}\,, \quad (4.1)$$

where the $\bar{\lambda}(0)$ depend on the strength of the applied forces. If the forces are switched off at time $t_0=0$ the distribution (4.1) will relax towards the equilibrium distribution $w(a)$. This relaxation is governed by the Fokker-Planck equation (2.1).

We want to study the time evolution of the mean values $\bar{a}(t)$ during this relaxation process. Since the $\bar{a}(t)$ are already determined by the "relevant part" $\bar{p}(a,t)$ of the distribution $p(a,t)$ we may eliminate the "irrelevant part" $\delta p(a,t)$ of the decomposition (3.9). This can be achieved by means of the projection-operator technique.[11] We define a projection operator $\mathcal{P}(t)$ by

$$\mathcal{P}(t)X(a)=\bar{p}(a,t)\mathrm{tr}X(a) + \frac{\partial\bar{p}(a,t)}{\partial\bar{a}^i(t)}\{\mathrm{tr}[a^iX(a)]-\bar{a}^i(t)\mathrm{tr}X(a)\}. \quad (4.2)$$

Note, that the time dependence of $\mathcal{P}(t)$ arises only through $\bar{p}(a,t)$ and, consequently, through the mean values $\bar{a}(t)$. We have from (3.4) and (3.5)

$$\mathrm{tr}\frac{\partial\bar{p}(a,t)}{\partial\bar{a}^j(t)}=0, \quad (4.3)$$

$$\mathrm{tr}\left(\frac{\partial\bar{p}(a,t)}{\partial\bar{a}^j(t)}a^i\right)=\delta^i_j. \quad (4.4)$$

Hence we find that $\mathcal{P}(t)$ fulfills

$$\mathcal{P}(t)\mathcal{P}(t')=\mathcal{P}(t), \quad (4.5)$$

which implies the projection-operator property for $t=t'$. Using (2.6) we see that $\mathcal{P}(t)$ projects out the relevant part $\bar{p}(a,t)$ of the distribution $p(a,t)$

$$\mathcal{P}(t)p(a,t)=\bar{p}(a,t), \quad (4.6)$$

so that the decomposition (3.9) may be written

$$p(a,t)=\mathcal{P}(t)p(a,t)+\mathcal{Q}(t)p(a,t) \quad (4.7)$$

where

$$\mathcal{Q}(t)=1-\mathcal{P}(t). \quad (4.8)$$

From (4.2) we have

$$\dot{\mathcal{P}}(t)X(a)=\frac{\partial^2\bar{p}(a,t)}{\partial\bar{a}^i(t)\partial\bar{a}^j(t)} \times\dot{\bar{a}}^j(t)\{\mathrm{tr}[a^iX(a)]-\bar{a}^i(t)\mathrm{tr}X(a)\}. \quad (4.9)$$

Hence we obtain

$$\dot{\mathcal{P}}(t)p(a,t)=0, \quad (4.10)$$

and, consequently,

$$\frac{\partial}{\partial t}\mathcal{P}(t)p(a,t)=\mathcal{P}(t)\frac{\partial}{\partial t}p(a,t). \quad (4.11)$$

Note that Eq. (4.11) does not hold if $p(a,t)$ is replaced by an arbitrary function of a and t. It is essential that the first moments of $p(a,t)$ are the mean values $\bar{a}(t)$ which give rise to the time dependence of $\mathcal{P}(t)$.

The Fokker-Planck equation (2.3) may be written

$$\frac{\partial}{\partial t}p(a,t)=\mathcal{L}p(a,t), \quad (4.12)$$

with the Fokker-Planck operator

$$\mathcal{L}X(a)=\frac{\partial}{\partial a^i}k_BL^{ij}(a)\left(\frac{\partial X(a)}{\partial a^j}-\frac{\partial w(a)}{\partial a^j}\frac{X(a)}{w(a)}\right) =\frac{\partial}{\partial a^i}\left(-K^i(a)+k_B\frac{\partial}{\partial a^j}D^{ij}(a)\right)X(a). \quad (4.13)$$

Using (4.6), (4.7), and (4.11) we have

$$\frac{\partial}{\partial t}\mathcal{Q}(t)p(a,t)=\mathcal{Q}(t)\mathcal{L}\bar{p}(a,t)+\mathcal{Q}(t)\mathcal{L}\mathcal{Q}(t)p(a,t), \quad (4.14)$$

which can be integrated to yield

$$\mathcal{Q}(t)p(a,t)=\int_0^t ds\,\mathcal{G}(t,s)\mathcal{Q}(s)\mathcal{L}\bar{p}(a,s), \quad (4.15)$$

where $\mathcal{G}(t,s)$ is the time-ordered exponential

$$\mathcal{G}(t,s)=T\exp\left(\int_s^t du\,\mathcal{Q}(u)\mathcal{L}\right) \quad (4.16)$$

in which operators are ordered from right to left as time increases. We have taken into account that the initial distribution is of the form (4.1) so that

$$p(a,0)=\bar{p}(a,0) \text{ or } \mathcal{Q}(0)p(a,0)=0. \quad (4.17)$$

Combining (4.6) and (4.15) we obtain from (4.7) an expression for $p(a,t)$ in terms of $\bar{p}(a,t)$ and its past history

$$p(a,t)=\bar{p}(a,t)+\int_0^t ds\,\mathcal{G}(t,s)\mathcal{Q}(s)\mathcal{L}\bar{p}(a,s). \quad (4.18)$$

If we insert this expression into (2.7) we find for the time rates of change of the mean values

$$\frac{d}{dt}\bar{a}^i(t)=\mathrm{tr}[K^i(a)\bar{p}(a,t)] +\int_0^t ds\,\mathrm{tr}[K^i(a)\mathcal{G}(t,s)\mathcal{Q}(s)\mathcal{L}\bar{p}(a,s)]. \quad (4.19)$$

Since the time dependence of $\bar{p}(a,t)$ and $\mathcal{Q}(t)$ arises only through $\bar{a}(t)$, so does the time dependence of $\mathcal{G}(t,s)$, and the right-hand side of Eq. (4.19) is completely determined by the mean values $\bar{a}(t)$ and their past history. Consequently, Eqs. (4.19) provide a closed set of equations of motion for the mean values. These are the "renormalized transport equations."

The transport equations (4.19) are not yet of the standard form where the fluxes are expressed in terms of transport coefficients and driving thermodynamic forces. In order to obtain this form, we make some transformations. With (2.4) and (3.6) we find

$$\mathrm{tr}[K^i(a)\bar{p}(a,t)] = \bar{L}_0^{ij}(t)\bar{\lambda}_j(t)\,, \tag{4.20}$$

where

$$\bar{L}_0^{ij}(t) = \mathrm{tr}[L^{ij}(a)\bar{p}(a,t)]\,. \tag{4.21}$$

Further, we obtain from (3.6) and (4.13)

$$\mathfrak{L}\bar{p}(a,t) = -\frac{\partial}{\partial a^i} L^{ij}(a)\bar{p}(a,t)\bar{\lambda}_j(t)\,, \tag{4.22}$$

so that

$$\mathrm{tr}[K^i(a)\,\mathcal{G}(t,s)\,\mathfrak{Q}(s)\mathfrak{L}\bar{p}(a,s)] = \bar{L}_1^{ij}(t,s)\lambda_j(s)\,, \tag{4.23}$$

where

$$\bar{L}_1^{ij}(t,s) = -\mathrm{tr}\left(K^i(a)\,\mathcal{G}(t,s)\,\mathfrak{Q}(s)\frac{\partial}{\partial a^k} L^{kj}(a)\bar{p}(a,s)\right). \tag{4.24}$$

Using (4.20) and (4.23) the renormalized transport equations (4.19) can be written

$$\frac{d}{dt}\bar{a}^i(t) = \bar{L}_0^{ij}(t)\bar{\lambda}_j(t) + \int_0^t ds\, \bar{L}_1^{ij}(t,s)\bar{\lambda}_j(s)\,. \tag{4.25}$$

These equations express the mean fluxes in terms of the renormalized thermodynamic forces $\bar{\lambda}$. There is not only an instantaneous reaction of the fluxes upon the momentary forces, but also a retarded reaction upon the forces at earlier times. Correspondingly, the "renormalized transport coefficients" $\bar{L}^{ij}$ consist of two parts. $\bar{L}_0^{ij}(t)$ describes the instantaneous transport. This coefficient is a function of the momentary mean values: $\bar{L}_0^{ij}(t) \equiv \bar{L}_0^{ij}(\bar{a}(t))$. The second part $\bar{L}_1^{ij}(t,s)$ describes the retarded transport caused by the forces at time $s<t$ and is a functional of the mean path in the time interval $[s,t]$:

$$\bar{L}_1^{ij}(t,s) \equiv \bar{L}_1^{ij}\{\bar{a}(u),\, s \le u \le t\}\,.$$

The equations (4.21) and (4.24) give exact expressions for the renormalized transport coefficients in terms of the bare transport coefficients $L^{ij}(a)$ and the bare entropy $S(a)$.

V. APPROXIMATE TRANSPORT EQUATIONS

So far we have made no approximations beyond those implicit in a Fokker-Planck model. As we have already mentioned, the Fokker-Planck equation (2.1) is often obtained from a more accurate equation by neglecting terms of higher order in a small parameter. In many cases we may look upon k_B as this small parameter, because it appears in the Fokker-Planck equation in the same way as the small parameter appears there. In such a case the Fokker-Planck equation must be viewed as an equation which is valid in order k_B only. Then it is also natural to neglect terms of more than first order in k_B in the renormalized transport equations. This approximation will be considered now.

A. Thermodynamic forces

Assume that the relevant distribution $\bar{p}(a,\bar{\lambda})$ has an absolute maximum at $a_0 = a_0(\bar{\lambda})$. From (3.8) we see that at the maximum

$$\left[\frac{\partial S}{\partial a^i}\right]_{a=a_0} = \bar{\lambda}_i\,. \tag{5.1}$$

We expand $S(a)$ about a_0. With

$$\Delta^i = a^i - a_0^i\,, \tag{5.2}$$

we have

$$S(a) = S_0 + S_i\Delta^i + \tfrac{1}{2}S_{ij}\Delta^i\Delta^j + \cdots\,, \tag{5.3}$$

where the Taylor coefficients

$$S_{i_1\cdots i_n} = \left[\frac{\partial^n S}{\partial a^{i_1}\cdots\partial a^{i_n}}\right]_{a=a_0} \tag{5.4}$$

are functions of $a_0(\bar{\lambda})$. With (5.1) and (5.3) the relevant distribution (3.8) may be written

$$\bar{p}(a,\bar{\lambda}) = N \times \exp[(1/k_B)(\tfrac{1}{2}S_{ij}\Delta^i\Delta^j + \tfrac{1}{6}S_{ijk}\Delta^i\Delta^j\Delta^k + \cdots)]\,, \tag{5.5}$$

where N is a normalization factor.

Let S^{ij} be the inverse[12] of the matrix S_{ij}

$$S^{ij}S_{jk} = S_{kj}S^{ji} = \delta_k^i\,, \tag{5.6}$$

and let $X(a)$ be an arbitrary state function with Taylor series about a_0 of the form

$$X(a) = X_0 + X_i\Delta^i + \tfrac{1}{2}X_{ij}\Delta^i\Delta^j + \cdots\,. \tag{5.7}$$

Then we obtain from (5.5)

$$\mathrm{tr}[\bar{p}(a,\bar{\lambda})X(a)] = X_0 + \tfrac{1}{2}k_B(X_i\gamma^i - X_{ij}S^{ij}) + O(k_B^2)\,, \tag{5.8}$$

where

$$\gamma^i = S^{ij}S^{kl}S_{jkl}\,. \tag{5.9}$$

Especially, we find for $X(a) = a^i$ that the mean value $\bar{a}^i$ reads

$$\bar{a}^i = a_0^i + \tfrac{1}{2}k_B\gamma^i + O(k_B^2)\,. \tag{5.10}$$

This relation determines $\bar{a}^i$ as of function of $a_0(\lambda)$. With (5.10) we obtain from (5.1)

$$\bar{\lambda}_i = \lambda_i(a_0) = \lambda_i(\bar{a}) - \tfrac{1}{2}k_B S_{ij}\gamma^j + O(k_B^2)\,. \tag{5.11}$$

Because of

$$\frac{\partial}{\partial a_0^i}\ln\|-S_{mn}\| = S_{mni}S^{mn} = S_{ij}\gamma^j\,, \tag{5.12}$$

where $\| \ \|$ denotes the determinant, the renormalized thermodynamic forces may be written

$$\bar{\lambda}_i(\bar{a}) = \frac{\partial \bar{S}(\bar{a})}{\partial \bar{a}^i}, \tag{5.13}$$

where

$$\bar{S}(\bar{a}) = S(\bar{a}) - k_B \ln \| -S_{mn}(\bar{a}) \|^{1/2} + O(k_B^2) \tag{5.14}$$

is the renormalized entropy in order k_B (up to an irrelevant constant).

B. Transport coefficients

From (4.21) we obtain with (5.8)

$$\bar{L}_0^{ij}(\bar{a}) = L^{ij}(a_0) + \frac{k_B}{2}\left(\frac{\partial L^{ij}(a_0)}{\partial a_0^k} \gamma^k - \frac{\partial^2 L^{ij}(a_0)}{\partial a_0^k \partial a_0^l} S^{kl} \right) + O(k_B^2), \tag{5.15}$$

which yields with (5.10)

$$\bar{L}_0^{ij}(\bar{a}) = L^{ij}(\bar{a}) - \frac{k_B}{2} \frac{\partial^2 L^{ij}(\bar{a})}{\partial \bar{a}^k \partial \bar{a}^l} S^{kl}(\bar{a}) + O(k_B^2). \tag{5.16}$$

This relation determines the instantaneous part of the renormalized transport coefficient in order k_B.

In order to determine the retarded part of the renormalized transport coefficient it is convenient to introduce the adjoint operator $\mathcal{L}^\dagger$ of the Fokker-Planck operator (4.13)

$$\mathcal{L}^\dagger X(a) = \left(K^i(a) \frac{\partial}{\partial a^i} + k_B D^{ij}(a) \frac{\partial^2}{\partial a^i \partial a^j} \right) X(a) = v^i(a) \frac{\partial}{\partial a^i} X(a) + O(k_B), \tag{5.17}$$

where

$$v^i(a) = L^{ij}(a) \frac{\partial S(a)}{\partial a^j}. \tag{5.18}$$

We also introduce the adjoint operator $\mathcal{P}^\dagger(t)$ of the projection operator (4.2):

$$\mathcal{P}^\dagger(t) X(a) = \mathrm{tr}[\bar{p}(a,t) X(a)] + [a^i - \bar{a}^i(t)] \mathrm{tr}\left(\frac{\partial \bar{p}(a,t)}{\partial \bar{a}^i} X(a) \right). \tag{5.19}$$

Then the expression (4.24) for the retarded part of the transport coefficient may be written

$$\bar{L}_1^{ij}(t,s) = -\mathrm{tr}\left(\xi^i(a,t,s)[1 - \mathcal{P}(s)] \frac{\partial}{\partial a^k} L^{kj}(a) \bar{p}(a,s) \right), \tag{5.20}$$

where $\xi^i(a,t,s)$ is given by

$$\xi^i(a,t,s) = \mathcal{G}^\dagger(s,t) K^i(a), \tag{5.21}$$

with the time-ordered exponential

$$\mathcal{G}^\dagger(s,t) = T_- \exp\left(\int_s^t du\, \mathcal{L}^\dagger [1 - \mathcal{P}^\dagger(u)] \right), \tag{5.22}$$

in which operators are ordered from left to right as time increases.

By the chain rule we have

$$\mathrm{tr}\left(\frac{\partial \bar{p}(a,\bar{\lambda})}{\partial \bar{a}^i} X(a) \right) = \frac{\partial a_0^k}{\partial \bar{a}^i} \frac{\partial}{\partial a_0^k} \mathrm{tr}[\bar{p}(a,\bar{\lambda}) X(a)]. \tag{5.23}$$

Further, (5.10) yields

$$\frac{\partial a_0^k}{\partial \bar{a}^i} = \delta_i^k - \frac{k_B}{2} \frac{\partial \gamma^k}{\partial a_0^i} + O(k_B^2). \tag{5.24}$$

If we insert (5.8) and (5.24) into (5.23), we obtain

$$\mathrm{tr}\left(\frac{\partial \bar{p}(a,\bar{\lambda})}{\partial \bar{a}^i} X(a) \right) = X_i + \tfrac{1}{2} k_B (X_{ij}\gamma^j + X_{jk} S^{jm} S^{kn} S_{imn} - X_{ijk} S^{jk}) + O(k_B^2). \tag{5.25}$$

Using (4.2), (5.8), and (5.25) we find

$$\mathrm{tr}\left(X(a)[1 - \mathcal{P}(\bar{\lambda})] \frac{\partial}{\partial a^i} L^{ij}(a) \bar{p}(a,\bar{\lambda}) \right) = -\tfrac{1}{2} k_B \Sigma^{j,mn} X_{mn} + O(k_B^2), \tag{5.26}$$

where the quantities on the right-hand side are taken at the position $a = a_0(\bar{\lambda})$, and where we have introduced

$$\Sigma^{j,mn} = \frac{\partial S^{mn}}{\partial a^p} L^{pj} - 2 S^{mp} \frac{\partial L^{nj}}{\partial a^p}. \tag{5.27}$$

The expression (5.20) for the retarded part of the renormalized transport coefficient coincides with the left-hand side of (5.26) for $X(a) = -\xi^i(a,t,s)$. Since the right-hand side of (5.26) is explicitly of order k_B, and since we neglect terms of higher order for the present consideration, we need to determine $\xi^i(a,t,s)$ for vanishing k_B only.

C. Transport coefficients, continued

Even in the limit $k_B \to 0$ the quantity $\xi^i(a,t,s)$ may still be a complicated nonlinear functional of $\{\lambda(u), s \le u \le t\}$. This functional can be expanded systematically in powers of $\bar{\lambda}$. For large times the system approaches the stationary state, which means that the $\bar{\lambda}$ approach 0. Hence we can often restrict ourselves to the first few terms of the expansion of ξ^i in powers of $\bar{\lambda}$. In the following, we shall neglect terms of the second order in $\bar{\lambda}$. This means that we disregard terms of the third order in $\bar{\lambda}$ in the transport equations, since these equations are already explicitly of first order in $\bar{\lambda}$.

Using (5.8), (5.10), and (5.25) we obtain from (5.19)

$$\mathcal{P}^\dagger(\bar\lambda)X(a)=X(a_0)+(a^i-a_0^i)\left[\frac{\partial X}{\partial a^i}\right]_{a=a_0}+O(k_B)\,, \tag{5.28}$$

where $a_0=a_0(\bar\lambda)$. Further, from (5.21) we see with (2.4), (5.17), (5.18), and (5.28) that the $k_B\to 0$ limit of $\xi^i(a,t,s)$ reads

$$\xi^i(a,t,s)=T_-\exp\left(\int_s^t du\,\mathcal{R}(u)\right)v^i(a)+O(k_B)\,. \tag{5.29}$$

The operator $\mathcal{R}(u)=\mathcal{R}(\bar\lambda(u))$ is defined by

$$\mathcal{R}(\bar\lambda)X(a)=v^i(a)\left(\frac{\partial X(a)}{\partial a^i}-\left[\frac{\partial X}{\partial a^i}\right]_{a=a_0}\right), \tag{5.30}$$

where $a_0=a_0(\bar\lambda)$. Expression (5.29) still contains all powers of $\bar\lambda$.

Now let a_m be the state where $S(a)$ takes its absolute maximum; i.e., $a_m=a_0(\bar\lambda=0)$. Then we have from (5.1) and (5.6)

$$a_0^i(\bar\lambda)=a_m^i+S^{ij}(a_m)\bar\lambda_j+O(\bar\lambda^2)\,, \tag{5.31}$$

which yields with (5.30)

$$\mathcal{R}(\bar\lambda)=\mathcal{R}_0+\mathcal{R}_1^i\bar\lambda_i+O(\bar\lambda^2)\,, \tag{5.32}$$

where

$$\mathcal{R}_0X(a)=v^i(a)\left(\frac{\partial X(a)}{\partial a^i}-\left[\frac{\partial X}{\partial a^i}\right]_{a=a_m}\right) \tag{5.33}$$

and

$$\mathcal{R}_1^iX(a)=-v^j(a)S^{ik}(a_m)\left[\frac{\partial^2 X}{\partial a^j\partial a^k}\right]_{a=a_m}. \tag{5.34}$$

By standard disentanglement of the time-ordered exponential in (5.29) we obtain

$$\xi^i(a,t,s)=e^{\mathcal{R}_0(t-s)}v^i(a)+\int_s^t du\,e^{\mathcal{R}_0(u-s)}\mathcal{R}_1^j e^{\mathcal{R}_0(t-u)}v^i(a)\bar\lambda_j(u)+O(\bar\lambda^2)\,. \tag{5.35}$$

Now, with (5.26), (5.31), and (5.35) the transport coefficient (5.20) takes the form

$$\bar L_1^{ij}(t,s)=\tfrac12 k_B\Sigma^{j,mn}\zeta^i_{mn}(t-s)+\tfrac12 k_B\Sigma^{j,mn}S^{kl}\zeta^i_{mnk}(t-s)\bar\lambda_l(s)+\tfrac12 k_B\frac{\partial\Sigma^{j,mn}}{\partial a^k}S^{kl}\zeta^i_{mn}(t-s)\bar\lambda_l(s)$$
$$-\tfrac12 k_B\int_s^t du\,\Sigma^{j,mn}S^{kl}\zeta^v_{mn}(u-s)\zeta^i_{vk}(t-u)\bar\lambda_l(u)+O(k_B^2)+O(\bar\lambda^2)\,, \tag{5.36}$$

where all a-dependent quantities are taken at the position $a=a_m$. The $\zeta^i(a,t)$ are defined by

$$\zeta^i(a,t)=e^{\mathcal{R}_0t}v^i(a)\,, \tag{5.37}$$

and we have introduced the quantities

$$\zeta^i_{mn}(t)=\left[\frac{\partial^2}{\partial a^m\partial a^n}\zeta^i(a,t)\right]_{a=a_m} \tag{5.38}$$

and

$$\zeta^i_{mnp}(t)=\left[\frac{\partial^3}{\partial a^m\partial a^n\partial a^p}\zeta^i(a,t)\right]_{a=a_m}. \tag{5.39}$$

Since a_m is a state where S has a maximum, we see from (5.18)

$$v^i(a_m)=0\,, \tag{5.40}$$

which yields with (5.33)

$$\mathcal{R}_0^2X(a)=\mathcal{L}_0^\dagger\mathcal{R}_0X(a)\,, \tag{5.41}$$

where

$$\mathcal{L}_0^\dagger X(a)=v^i(a)\frac{\partial X(a)}{\partial a^i}\,. \tag{5.42}$$

Further, we obtain with (5.33) and (5.42)

$$\mathcal{R}_0v^i(a)=\mathcal{L}_0^\dagger(v^i(a)-M^i_ja^j)\,, \tag{5.43}$$

where

$$M^i_j=\left[\frac{\partial v^i}{\partial a^j}\right]_{a=a_m}. \tag{5.44}$$

Using (5.41) and (5.43) we see that (5.37) may be transformed to yield

$$\zeta^i(a,t)=M^i_ja^j+e^{\mathcal{L}_0^\dagger t}[v^i(a)-M^i_ja^j]\,. \tag{5.45}$$

We now make use of the relation

$$\left[\frac{\partial}{\partial a^i}e^{\mathcal{L}_0^\dagger t}X(a)\right]_{a=a_m}=0\,,\quad\text{for}\quad\left[\frac{\partial X}{\partial a^i}\right]_{a=a_m}=0\,. \tag{5.46}$$

This relation is a consequence of (5.40) and (5.42). In the power series expansion of the exponential the derivatives $\partial/\partial a^i$ of an operator $\mathcal{L}_0^\dagger$ must act upon the drift vector $v^i(a)$ of the next operator $\mathcal{L}_0^\dagger$ to the right in order that we obtain a nonvanishing result.

Using (5.45) and (5.46) we obtain from (5.38) and (5.39)

$$\frac{d}{dt}\zeta^i_{mn}(t)=M^k_m\zeta^i_{kn}(t)+M^k_n\zeta^i_{mk}(t)\,, \tag{5.47}$$

$$\frac{d}{dt}\zeta^i_{mnp}(t)=M^k_m\zeta^i_{knp}(t)+M^k_n\zeta^i_{mkp}(t)+M^k_p\zeta^i_{mnk}(t)+M^k_{mn}\zeta^i_{kp}(t)+M^k_{np}\zeta^i_{km}(t)+M^k_{mp}\zeta^i_{nk}(t)\,, \tag{5.48}$$

where

$$M^k_{mn}=\left[\frac{\partial^2 v^k}{\partial a^m \partial a^n}\right]_{a=a_m} . \quad (5.49)$$

Equation (5.47) must be solved with the initial condition

$$\zeta^i_{mn}(0)=M^i_{mn} . \quad (5.50)$$

If the solution of (5.47) is known, we can look upon (5.48) as an inhomogeneous equation for $\zeta^i_{mnp}(t)$ with known inhomogeneity. The initial condition reads

$$\zeta^i_{mnp}(0)=\left[\frac{\partial^3 v^i}{\partial a^m \partial a^n \partial a^p}\right]_{a=a_m} . \quad (5.51)$$

This shows that we can avoid to solve a nonlinear first-order partial differential equation to determine $\zeta^i(a,t)$, rather we need only to solve the much simpler linear equations (5.47) and (5.48) in order to determine the renormalized transport coefficient in the approximation under consideration. Note that the approximation (5.36) for the retarded part of the renormalized transport coefficients already goes beyond the lowest nontrivial order. In the lowest approximation we may completely neglect the dependence of the renormalized transport coefficients on the thermodynamic forces $\bar{\lambda}$ since the transport equations (4.25) are already explicitly of first order in $\bar{\lambda}$. In this case we must only solve Eqs. (5.47).

The next order in λ leads to the equations (5.48). The approximation scheme outlined above can be carried out in a systematic way to determine corrections of higher order in k_B as well as corrections of higher order in $\bar{\lambda}$. Naturally, since we made no assumptions about the nonlinearities, every higher-order approximation contains new vertices in general. For every system with specific nonlinearity the specific higher-order corrections are much more easily worked out than their general form, and the way in which these corrections may be obtained is clear from previous considerations.

VI. CONCLUSION

We have derived fully fluctuation-renormalized transport equations for a fluctuating thermodynamic system whose dynamics is governed by a nonlinear Fokker-Planck equation. The transport equations are valid in every time regime. They are particularly favorable to discuss the long-time limit where nonlinear terms in the renormalized thermodynamic forces $\bar{\lambda}$ can be neglected. However, the basic equations (4.25) also describe the dynamics of the mean values in the initial time period when the system may be in the nonlinear regime far from equilibrium.

It is well known that statistical mechanics generally leads to a non-Markovian stochastic process for the macroscopic variables. The Markovian assumption upon which we have based our considerations requires a small parameter controlling the Markovian limit, and we have introduced Boltzmann's constant k_B as a general substitutional parameter. This is a natural procedure for systems which relax towards thermal equilibrium, and we have explained the theory within this framework. However, apart from some simple changes, our analysis applies to other systems governed by a nonlinear Fokker-Planck equation.

We have obtained closed analytical expressions for the renormalized thermodynamic forces and the renormalized transport coefficients in terms of the corresponding bare quantities. To evaluate those expressions approximately we discussed their systematic expansion in powers of k_B and $\bar{\lambda}$. The crucial assumption upon which we have based the outlined approximation scheme is that the entropy $S(a)$ should have an absolute maximum at a state a_m where the matrix of the second-order derivatives $\partial^2 S/\partial a^i \partial a^j$ is nonsingular. This means that the statics of the system is noncritical. Examples where these assumptions hold have been discussed by others,[13] and their results can easily be obtained from our approximate equations. If the static distribution does not meet these assumptions, the exact form (4.25) of the transport equations is still valid but the approximation scheme must be altered. A possible strategy for a bistable system has been put forward recently.[14]

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