Continously Perturbed Equivalent Classes of Asymptotically Stable Kinetic Equations

I. Stochastic Perturbations with Coefficient Dependent on the Macrostate

A. D. NAZAREA*

Faculté des Sciences de l'Université Libre de Bruxelles

(Z. Naturforsch. **28a**, 305–308 [1973]; received 25 August 1972)

Equivalent classes of kinetic (rate) equations for which each class is asymptotically stable with respect to a unique steady-state are assumed subject to a multi-dimensional stochastic pertubation arising as the time derivative of a vector-valued normalized Wiener process. A general condition for stability of the steady-state, *with probality one*, under such continously acting random perturbations is derived in terms of the kinetic potential. An application of this condition is given in the appendix.

I. Introduction

In a series of recent papers[1, 2, 3] a constructive theory was developed to generate asymptotically stable equivalent classes of kinetic (rate) equations possessing, for each class, a unique steady-state. These equivalent classes are generated by *stability constraint specifications*, discussed briefly in the next section.

The present work is an attempt to derive a *selfcontained* condition for the stability behavior of these equivalent classes under continuously acting multidimensional random perturbation, on the assumption that the perturbation can be regarded as the time derivative of a vector-valued normalized Wiener process with independent components—in other words, generalized multi-component Gaussian noise or Langevin pertubation—and with coefficient matrix dependent on the macrostate. By a self-contained condition is meant one that can be expressed in terms of the kinetic potential associated with the equivalent class and of the coefficient matrix of the stochastic perturbation. Such a condition is derived using recent results in the stability analysis of stochastic dynamical systems[4, 5].

II. The Unpertubed Equivalent Classes

We were concerned in (A) with the open set $\Omega_{(n)}$ in the space of the macrovariable $\boldsymbol{Q}$,

$$\Omega_{(n)} \equiv \{\boldsymbol{Q} \mid \boldsymbol{Q} > \boldsymbol{0}\}$$

where $\boldsymbol{Q}$, e.g. particle numbers or concentrations, is a column n-vector, with $n < \infty$. There, attention was restricted to all equivalent classes of kinetic equations defined in $\Omega_{(n)}$ which have, for each class, a unique steady-state, denoted by $\boldsymbol{\sigma}$, belonging to $\Omega_{(n)}$. Owing to this restriction, it is possible to transform to Onsager coordinates (pertubed coordinates) thus: $\mathbf{x} \equiv \boldsymbol{Q} - \boldsymbol{\sigma}$; that is to say, in terms of derviations fom the steady-state. In the space of Onsager coordinates, the open set $\Omega_{(n)}$ has the representation

$$\Omega_{(n)} \equiv \{\mathbf{x} \mid \mathbf{x} > -\boldsymbol{\sigma}\}. \tag{2.1}$$

In the sequal, when reference is made to $\Omega_{(n)}$, (2.1) will be meant.

It is clear that in $\Omega_{(n)}$ the point $\mathbf{x} = \mathbf{0}$ corresponds to the steady-state. Consequently, in generating the exhaustive equivalent classes of asymptotically stable kinetic equations having a unique steady-state for each class, it is sufficient to generate all those for which $\mathbf{x} = \mathbf{0}$ is the only positively invariant set for the flux[1, 2]. The constructive approach followed in (A) is through a stability constraint specification. Such a specification, when well-posed, consists of: (i) a generalized positive-definite kinetic potential[6] $V(\mathbf{x})$ mapping $\Omega_{(n)}$ to the reals, at least twice continously differentiable, strictly convex in $\Omega_{(n)}$ and radially unbounded; (ii) a scalar real-valued continous function $\xi(\mathbf{x})$, positive-definite in $\Omega_{(n)}$, the absolute value of which specifies the total time rate of decrescence of the kinetic potential along the reaction trajectory,

$$\dot{V}(\mathbf{x}) = -\xi(\mathbf{x}). \tag{2.2}$$

It is shown in (A) that if $\mathbf{x} = \mathbf{0}$ is indeed the isolated global minimum of the kinetic potential in $\Omega_{(n)}$, the exhaustive equivalent classes of kinetic equations generated by the constraint specification will have its unique steady-state at this minimum point. This is assured by strict convexity of the kinetic potential — which is equivalent to the condition that the Hessian matrix $\boldsymbol{H}_V(\mathbf{x})$ of this potential possess a positive spectrum of eigenvalues in $\Omega_{(n)}$ — together with the vanishing of its gradient vector at this point and at this point alone. Furthermore, it is shown in (A) that these equivalent classes will have flux equations of the general form

$$\mathbf{J}(\mathbf{x}) \equiv \mathrm{d}\mathbf{x}/\mathrm{d}t = \boldsymbol{U}(\mathbf{x}) \operatorname{grad} V(\mathbf{x}) \tag{2.3}$$

with $\boldsymbol{U}(\mathbf{x}) \equiv \operatorname{diag}(\beta(\mathbf{x})) + \mathbf{W}(\mathbf{x})$,

* Present address: Center for Statistical Mechanics and Thermodynamics, The University of Texas at Austin, Austin 78712/U.S.A.

where $\mathbf{W}(\mathbf{x})$ is a continous n-dimensional real skew-symmetric matrix and the n-dimensional diagonal matrix has elements

$$\beta(\mathbf{x}) = -\xi(\mathbf{x})/\|\text{grad } V(\mathbf{x})\|^2, \tag{2.4}$$

the symbol $\|\cdot\|$ denoting the Euclidean norm. The particular flux equation of any one member of an equivalent glass is generated by the choice of $\mathbf{W}(\mathbf{x})$.

Due to the properties of the kinetic potential, or more precisely, of the stability constraint specification, any reaction trajectory generated by (2.3) is unique, given any initial state in $\Omega_{(n)}$, the flux being always a Lipschitz function; furthermore, this trajectory is globally extendable for positive time and hence defines a commutative semi-group of continuous transformations parametrized by (positive) time.

The above-cited work [2] should be consulted for the detailed development of the theory, which enables one to calculate, for instance, given an initial fluctuation $\mathbf{x}_0$ from the steady-state, the upper bound for the generalized relaxation time of the fluctuation.

III. The Randomly Pertubed Equivalent Classes

Consider now the flux Eq. (2.3) subjected to an m-dimensional random vector perturbation $\boldsymbol{r}(t)$, $m \leq n$, such that

$$\mathbf{J}^s(\mathbf{x}) = \boldsymbol{U}(\mathbf{x}) \text{ grad } V(\mathbf{x}) + \boldsymbol{G}(\mathbf{x})\boldsymbol{r}(t). \tag{3.1}$$

The $n \times m$ coupling matrix $\boldsymbol{G}(\mathbf{x})$ depends on the macrostate, and will be required to be continuous, with $\boldsymbol{G}(\mathbf{0}) = \mathbf{0}$.

It will be assumed that the random perturbation $\boldsymbol{r}(t)$ arises as the time derivativ of a vector-valued m-dimensional normalized Wiener process $\boldsymbol{w}(t)$ with independent components:

$$\boldsymbol{w}(t) = \int_0^t \boldsymbol{r}(\bar{\tau})\mathrm{d}\bar{\tau}. \tag{3.2}$$

This mathematically unambiguous assumption is equivalent to the more physically familiar one [7] that $\boldsymbol{r}(t)$ is an m-dimensional Gaussian noise vector or Langevin-type perturbation. Using (3.2), the flux equations can be written more precisely in Itô form thus:

$$\mathbf{J}^s(\mathbf{x})\mathrm{d}t \equiv \mathrm{d}\mathbf{x}(t) = \boldsymbol{U}(\mathbf{x}) \text{ grad } V(\mathbf{x}) \,\mathrm{d}t + \boldsymbol{G}(\mathbf{x})\,\mathrm{d}\boldsymbol{w}(t). \tag{3.3}$$

The solution $\mathbf{x}(t)$ of this equation defines a vector-valued stochastic process.

It remains now to find conditions, if possible in terms of the kinetic potential alone, which assure that for this stochastic process, given an initial state belonging to $\Omega_{(n)}$, the steady-state is stable *with probability one.*

IV. Stochastic Stability Conditions in Terms of the Constraint Specification

We observe that given, on the one hand, the continuity of $\boldsymbol{U}(\mathbf{x})$ and the properties of the kinetic potential, which assure the global positive extendability in $\Omega_{(n)}$ of the unperturbed reaction trajectory defined by the flux equation (2.3), and the continuity of $\boldsymbol{G}(\mathbf{x})$ with $\boldsymbol{G}(\mathbf{0}) = \mathbf{0}$ on the other, these conditions are sufficient to assure that the vector-valued stochast processic $\mathbf{x}(t)$ defined by (3.3) or (3.1) is, with probability one, a *right-continuous strong Markov process* [4,5] for any initial state $\mathbf{x}_0$ belonging to $\Omega_{(n)}$ and all $t < \infty$. We shall rely on the results of the last cited works for our subsequent analysis

The *weak infinitesimal operator* of the strong Markov process $\mathbf{x}(t)$ will be denoted by $\mathscr{A}_\Omega$. Since the kinetic potential is twice continuously differentialbe in $\Omega_{(n)}$, it processes a continuous Hessian matrix $\boldsymbol{H}_V(\mathbf{x})$ for all $\mathbf{x}$ belonging to $\Omega_{(n)}$. Consequently, the kinetic potential is in the domain of the weak infinitesimal operator of the process $\mathbf{x}(t)$, and we have

$$\mathscr{A}_\Omega[V(\mathbf{x})] = \langle \text{grad } V(\mathbf{x}), \mathbf{J}(\mathbf{x})\rangle + \tfrac{1}{2}\Sigma_{ij} \Lambda_{ij}(\mathbf{x}) H_V^{ij}(\mathbf{x}), \tag{4.1}$$

where $\quad \boldsymbol{\Lambda}(\mathbf{x}) = \boldsymbol{G}(\mathbf{x})\boldsymbol{G}^{\mathrm{T}}(\mathbf{x}).$

Now the first term on the right hand sincle of (4.1) is, from (2.2), just $-\xi(\mathbf{x})$ of the stability constraint specification; and hence, using (2.4), one can rewrite (4.1) as

$$\mathscr{A}_\Omega[V(\mathbf{x})] = \beta(\mathbf{x}) \|\text{grad } V(\mathbf{x})\|^2 + \tfrac{1}{2}\Sigma_{ij} \Lambda_{ij}(\mathbf{x}) H_V^{ij}(\mathbf{x}), \tag{4.2}$$

$i, j = 1, \ldots, n$. It is clear that if the relation

$$\tfrac{1}{2}\Sigma_{ij} \Lambda_{ij}(\mathbf{x}) H_V^{ij}(\mathbf{x}) \leq -\beta(\mathbf{x}) \|\text{grad } V(\mathbf{x})\|^2 \tag{4.3}$$

were to hold, the kinetic potential is a *non-negative supermartingale* of the strong Markov process $\mathbf{x}(t)$. But this is exactly what is required if one wants to make a statement, with probability one, about the stochastic stability of $\mathbf{x}(t)$ with respect to the steady-state in terms of the kinetic potential, or more generally, of the constraint specification. Thus, (4.3) furnishes a self-contained condition as defined in the Introduction, being dependent only on the Hessian matrix and the gradient vector of the kinetic potential and the coefficient matrix of the stochastic perturbation, and of course, implicitly, on the scalar function $\xi(\mathbf{x})$ of the constraint specification

Note finally that the specification of $\xi(\mathbf{x})$ usually takes the general functional form

$$\xi(\mathbf{x}) = f[\mathbf{x}; \|\text{grad } V(\mathbf{x})\|];$$

while in the simplest examples in (A), corresponding to the cases in which the diagonal elements of $\boldsymbol{U}(\mathbf{x})$ are negative constant sequal, say, to $-k$, it is taken as

$$\xi(\mathbf{x}) = k \|\text{grad } V(\mathbf{x})\|^2. \tag{4.4}$$

For these cases, the condition (4.3) reducts to

$$\tfrac{1}{2}\Sigma_{ij} \Lambda_{ij}(\mathbf{x}) H_V^{ij}(\mathbf{x}) \leq k \|\text{grad } V(\mathbf{x})\|^2.$$

V. Summary

A well-posed stability constraint specification involving a generalized kinetic potential and its (total time rate of decrescence generates an equivalent class of flux equations of the form (2.3). We have considered here the problem of finding a self-contained condition (one mainly involving the kinetic potential and its rate of time decrescence) for stochastic stability when (2.3) is perturbed by a multi-dimensional stochastic process which can be considered as the time derivative of a vector-valued normalized Wiener process with independent components, as in (3.3) or (3.1). Given that the stability constraint specification is wellposed and certain conditions on the coupling matrix of the stochastic perturbation are met, the stochastic process $\mathbf{x}(t)$ corresponding to the solution of (3.3) is a right-continuous strong Markov process. The negative-definiteness of the weak infinitesimal operator of $\mathbf{x}(t)$ — which can be expressed in terms of the Hessian and gradient vector of the kinetic potential — assures that this potential is a non-negative supermartingale of the process, and furnishes the condition for stochastic stability: The right-continuous strong Markov process $\mathbf{x}(t)$ corresponding to the reaction trajectory of 3.2) is stable with respect to the steady-state, *with probability one*, whenever the constraint specification satisfies the subsidiary condition

$$\frac{\frac{1}{2}\Sigma_{ij}A_{ij}(\mathbf{x})\,H_V^{ij}(\mathbf{x})}{-\beta(\mathbf{x})\,\|\text{grad}\,V(\mathbf{x})\|^2}\leq 1 \tag{5.1}$$

in $\Omega_{(n)}$.

Acknowledgements

I should like to thank Professor I. PRIGOGINE and Professor G. NICOLIS for their kind interest. This work was undertaken with the support of the Fonds de la Recherche Fondamentale Collective.

Appendix

Here we indicate a simple application of the results derived in the text, namely to the equivalent class of flux equations to which belongs every classical Onsager-Machlup system.

Proposition: Consider the unperturbed equivalent class of kinetic equations which is generated by a stability constraint specification consisting of (i) a *quadratic* kinetic potential

$$V(\mathbf{x}) = \tfrac{1}{2}\langle\mathbf{x}, C\,\mathbf{x}\rangle, \tag{A.1}$$

C being a real symmetric n-dimensional positive-definite matrix, and (ii) a total time rate of decrescence of the kinetic potential (along the flux trajectory) which is proportional to the square of the norm of its gradient vector, as in (4.4):

$$\dot{V}(\mathbf{x}) = -\,\xi(\mathbf{x}) = -k\,\|\text{grad}\,V(\mathbf{x})\|^2, \tag{A.2}$$

$k > 0$.

Let the equations belonging to the equivalent class thus generated be subject to a multi-dimensional stochastic perturbation $\boldsymbol{R}(t)$ of the form

$$\boldsymbol{R}(t) = \boldsymbol{G}(\mathbf{x})\,\boldsymbol{r}(t), \tag{A.3}$$

where $\boldsymbol{r}(t)$ is the derivativ of a normalized n-dimensional Wiener process and where the coefficient matrix of the perturbation is diagonal,

$$\boldsymbol{G}(\mathbf{x}) = \text{diag}(\text{g}(\mathbf{x})), \tag{A.4}$$

with $g(\mathbf{0}) = 0$, then the equivalent class is stable with respect to the steady-state $\mathbf{x} = \mathbf{0}$ under the continuously acting perturbations (A.3), with probability one, if $g(\mathbf{x})$ satisfies the upper bound condition

$$\text{g}(\mathbf{x}) \leq \left[\frac{2k\,\mathbf{x}^{\mathrm{T}}C^{\mathrm{T}}C\,\mathbf{x}}{\text{tr}\,C}\right]^{1/2} \tag{A.5}$$

Remarks: (i) For the present example, the unperturbed flux Eq. (2.3) for the equivalent class is given by

$$\mathbf{J}(\mathbf{x}) = [\text{diag}(-k) + \mathbf{W}(\mathbf{x})]\,\text{grad}\,V(\mathbf{x}) \tag{A.6}$$

and each member of the equivalent class is generated by a particular choice of the real skew-symmetric matrix $\mathbf{W}(\mathbf{x})$. The continuously pertubed flux equation is then

$$\mathbf{J}^s(\mathbf{x}) = [\text{diag}(-k) + \mathbf{W}(\mathbf{x})]\,C\mathbf{x} + \text{diag}(\text{g}(\mathbf{x}))\,\boldsymbol{r}(t) \tag{A.7}$$

(ii) Forgetting for the moment the fact that a different type of stochastic perturbation is involved in (A.7) than was originally assumed by ONSAGER and MACHLUP[8, 9], we see that classical Onsager-Machlup systems are imbedded as *one* subclass (indeed the *simplest* subclass) of the equivalent class defined by (A.6), if the formal kinetic potential is viewed as entropy. This becomes clear if considered in the following way. One can choose $\mathbf{W}(\mathbf{x})$ to be independent of the macrostate, *i.e.*, $\mathbf{W}(\mathbf{x}) = \mathbf{W}$, from which choice one can rewrite (A.6) as

$$\mathbf{J}(\mathbf{x}) = -\,[\text{diag}(k) + \mathbf{W}]\,C\,\mathbf{x}, \tag{A.8}$$

where $\mathbf{W} = \widetilde{\mathbf{W}}$, another skew-symmetric matrix. Note that the matrix $[\text{diag}(k) + \widetilde{\mathbf{W}}]\,C$ has eigenvalues with positive real parts. In order to generate the subclass of classical Onsager-Machlup systems considered in Ref. 8 for instance, it is necessary to restrict consideration to macrovariables $\mathbf{x}$ all of whose components posses *even* parity with respect to time reversal. For this it is necessary and sufficient to require that $\widetilde{\mathbf{W}}$ be chosen so as to make $[\text{diag}(k) + \widetilde{\mathbf{W}}]\,C$ symmetric. All members of the subclass are then generated by all possible choices of the symmetric positive-definite matrix C defining their kinetic potential.

In the next paper of the series, we shall consider the case of quadratic kinetic potentials separately and in greater detail[10].

Proof of the Proposition: The assertion of the proposition follows at once from the general condition derived in the text. Frow (A.4),

$$\Lambda(\mathbf{x}) = \text{diag}\,[(g(\mathbf{x}))^2]. \tag{A.9}$$

By taking note of this, and of the fact that the gradient vector of the quadratic potential is simply

$$\text{grad}\, V(\mathbf{x}) = \boldsymbol{C}\,\mathbf{x},$$

with Hessian matrix

$$\boldsymbol{H}_V(\mathbf{x}) = \boldsymbol{C},$$

then, in view of (2.4) and the constraint specification (A.1) and A.2) generating the equivalent class, the condition (5.1) reduces to

$$\frac{\frac{1}{2}(g(\mathbf{x}))^2\,\text{tr}\,\boldsymbol{C}}{k\,\|\boldsymbol{C}\mathbf{x}\|^2} \leq 1 \tag{A.10}$$

from which (A.5) follows directly. Thus $g(\mathbf{x})$ must be bounded by the square root of a certain positive-definite quadratic form. That this upper bound condition for $g(\mathbf{x})$ can be expressed in terms of the kinetic potential (A.1) is seen by noting that

$$\mathbf{x}^{\mathrm{T}}\boldsymbol{C}^{\mathrm{T}}\boldsymbol{C}\,\mathbf{x} = V(\mathbf{x}) + \mathbf{x}^{\mathrm{T}}\widetilde{\boldsymbol{C}}\,\mathbf{x}$$

where $\widetilde{\boldsymbol{C}} = (\boldsymbol{C}^{\mathrm{T}} - \boldsymbol{I})\,\boldsymbol{C}$.

1 A.D. NAZAREA and S.A. RICE, Proc. Nat. Acad. Sci. USA **68**, 2502 [1971].
2 A.D. NAZAREA, Biophysik **8**, 96 [1972]. Referred to as (A).
3 A.D. NAZAREA, **ibid.**, **9**, 93 [1973].
4 H.J. KUSHNER, Proc. Nat. Acad. Sci. USA **53**, 8 [1965].
5 H.J. KUSHNER, Stochastic Stability and Control, Academic Press, New York 1967.
6 The notion of a kinetic potential was first studied by Prigogine and co-workers; for a summary, see P. GLANSDORFF and I. PRIGOGINE, Thermodynamic of Structure, Stability and Fluctuations, Wiley-Intersience, London 1971. The kinetic potential they have introduced differs in some respects from the potential introduced in (A) on account of the constructive approach adopted in the latter through the concept of a stability constraint specification; this approach assures, among other things, that the 'generalized kinetic potential' always exists.
7 M.C. WANG and G.E. UHLENBECK, Rev. Mod. Phys. **17**, 323 [1945].
8 L. ONSAGER and S. MACHLUP, Phys. Rev. **91**, 1505 [1953].
9 S. MACHLUP and L. ONSAGER, Phys. Rev. **91**, 1512 [1953].
10 A.D. NAZAREA, Molec. Phys. **25**, 1061 [1973].