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Brownian Motion on a Manifold

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The question of the existence and correct form of equations describing Brownian motion on a manifold cannot be answered by mathematics alone, but requires a study of the underlying physics. As in classical mechanics, manifolds enter through the transformation of variables needed to account for the presence of constraints. The constraints are either due to a physical agency that forces the motion to remain on a manifold, or they represent conserved quantities of the equation of motion themselves. Also the Brownian motion is described either by a Smoluchowski diffusion equation or by a Kramers equation. The four cases lead to the following conclusions. (i) Smoluchowski diffusion with a conserved quantity reduces to a diffusion equation on the manifold; (ii) The same is true for diffusion with a physical constraint in three dimensions, but in more dimensions it may happen that *no* autonomous equation on the manifold results; (iii) A Kramers equation with a conserved quantity reduces to an equation on the manifold, but in general not of the form of a Kramers equation; (iv) The Kramers equation with a physical constraint reduces to an autonomous Kramers equation on the manifold only for a special shape of that constraint. Throughout, only a certain type of physical constraints has been envisaged, and global questions are ignored. Finally, the customary heuristic construction of a Fokker–Planck equation for a mechanical system on a manifold is demonstrated for the case of Brownian rotation of a rigid body, and its shortcomings are emphasized.

KEY WORDS: Brownian motion; diffusion; Kramers equation; constraints; manifolds.

1. INTRODUCTION

Newtonian mechanics deals with particles subject to mutual and external forces obeying the equations

$$\dot{\mathbf{r}}_n = \mathbf{p}_n/m_n \qquad \dot{\mathbf{p}}_n = \mathbf{f}_n(\mathbf{r}, \mathbf{p})$$

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(Throughout we restrict ourselves to equations that are invariant for time translation: external forces must be constant in time.) The $\mathbf{r}_n$ are cartesian coordinates in an euclidean configuration space. In the presence of connecting rods, guiding surfaces, etc., the equations have to be modified to take into account the effect of these constraints, as was done by d'Alembert.[1] When the constraints are holomic they restrict the motion to a submanifold $\mathbb{M}$ of configuration space, so that the set of coordinates $\mathbf{r}_n$ is redundant. Lagrange[2] has shown how to transform to a smaller set of variables q_k, which describe the motion on $\mathbb{M}$. They are coordinates on $\mathbb{M}$ and in general not Cartesian. A large part of modern mechanics is devoted to the study of the motion on such manifolds.[3]

Such constraints are idealized descriptions of the elastic forces in the rods, etc.,[4] and we call them *physical constraints*. Another type occurs when the equations themselves have one or more conserved quantities

$$\Phi(\mathbf{r}, \dot{\mathbf{r}}) = c \tag{1}$$

Then the motion is *automatically* confined to the submanifold in phase space determined by (1). It is again possible to utilize this fact by transforming to a smaller set of variables. Dirac[5] has created confusion by using the name constraint also for such constants of the motion; we call them *mathematical constraints.*

Remark. In nonmechanical Lagrange problems it may happen that the Lagrange function $L(q, \dot{q})$ is singular,[6] in the sense that

$$\operatorname{Det} \frac{\partial^2 L}{\partial \dot{q}_k \, \partial \dot{q}_l} = 0$$

Then the momenta p_k are not independent functions of the velocities $\dot{q}_l$, but instead there exists an identity

$$\Omega\left(\frac{\partial L}{\partial \dot{q}_k}, q\right) = 0 \tag{2}$$

It has the same form as (1), but the constant c now has one definite value. This type of mathematical constraint will occur in Section 5.

Now suppose that the particles of our system are subject to dissipation and therefore also to fluctuations. Then it may be described by a set of coupled Langevin equations, or by the equivalent Fokker–Planck equation

$$\frac{\partial P(x, t)}{\partial t} = -\frac{\partial}{\partial x^i} A^i(x) \, P + \frac{1}{2} \frac{\partial^2}{\partial x^i \, \partial x^j} B^{ij}(x) \, P \tag{3}$$

The x^i are the Cartesian coordinates of the particles and may also comprise their momenta (Section 4). They identify the instantaneous state of the system as a point in a d-dimensional space $\mathbb{R}^d$ and summation is implied. The coefficients A^i, B^{ij} embody the properties of the system and are known functions of x. For each x the matrix B^{ij} is symmetric and nonnegative semidefinite. The motion of the system is now a Markov process whose transition probability $P(x, t \mid x_0, t_0)$ (from the state x_0 at t_0 into x at t) is that solution of (3) that is singled out by

$$P(x, t_0) = \delta(x - x_0)$$

Again it may happen that the motion is confined to a submanifold in $\mathbb{R}^d$, either by a physical or by a mathematical constraint. An example of a *physical* constraint is Brownian motion in a thin sheet between two impenetrable surfaces (Sections 3 and 6). A *mathematical* constraint occurs when the A^i and B^{ij} in (3) are such that there exists a conserved quantity $\Phi(x)$. In either case the motion is confined to a submanifold $\mathbb{M}$ and our aim is to obtain an equation in a reduced set of variables that describes the stochastic motion on $\mathbb{M}$.

Brownian motion on a manifold has been studied in the mathematical literature.[7] However, there the problem is the connection between the Langevin equation and the diffusion for a system confined to a manifold, rather than the validity of the equations for physical systems. Our strategy is to start from the known equations for Brownian motion in Cartesian coordinates and subsequently investigate the effect of the constraints, either mathematical or physical, which are responsible for confining the system to a manifold.

In physics, Brownian motion on a manifold has been studied mainly in connection with the Brownian rotation of molecules.[8,9] The Euler angles are parameters on a three-dimensional $\mathbb{M}$ and one constructs a Fokker–Planck equation on $\mathbb{M}$ heuristically. In our last section we sketch this approach and indicate its shortcomings, without however being able as yet to provide a more satisfactory derivation in accordance with the strategy mentioned above.

2. FOKKER–PLANCK EQUATION WITH CONSERVED QUANTITIES

An essential ingredient is the general transformation of the Fokker–Planck equation (3) to new variables $\bar{x}^k = \bar{x}^k(x)$. The probability density in the new variables is

$$\bar{P}(\bar{x}, t) = P(x, t) \left| \operatorname{Det} \frac{\partial \bar{x}^k}{\partial x^i} \right|^{-1} \tag{4a}$$

It obeys a Fokker–Planck equation of the same form (3) with the new coefficients[9,10]

$$\bar{A}^k = A^i \frac{\partial \bar{x}^k}{\partial x^i} + \frac{1}{2} B^{ij} \frac{\partial^2 \bar{x}^k}{\partial x^i \, \partial x^{i}}, \qquad \bar{B}^{kl} = B^{ij} \frac{\partial \bar{x}^k}{\partial x^i} \frac{\partial \bar{x}^l}{\partial x^j} \tag{4b}$$

A quantity $\Phi(x)$ is conserved by (3) if not only its average, but all its moments, are constant, that is, if for every function $f(\cdot)$

$$0 = \frac{d}{dt} \int f(\Phi) \, P \, dx = \int f[\Phi(x)] \frac{\partial P(x, t)}{\partial t} \, dx$$

$$= \int P \, dx \left\{ A^i \frac{\partial \Phi}{\partial x^i} f'(\Phi) + \frac{1}{2} B^{ij} \left[\frac{\partial^2 \Phi}{\partial x^i \, \partial x^j} f'(\Phi) + \frac{\partial \Phi}{\partial x^i} \frac{\partial \Phi}{\partial x^j} f''(\Phi) \right] \right\}$$

The coefficients of f'' and f' must vanish separately

$$B^{ij} \frac{\partial \Phi}{\partial x^i} \frac{\partial \Phi}{\partial x^j} = 0, \qquad A^i \frac{\partial \Phi}{\partial x^i} + \frac{1}{2} B^{ij} \frac{\partial^2 \Phi}{\partial x^i \, \partial x^j} = 0 \tag{5a}$$

As B^{ij} is semidefinite the first condition is equivalent with

$$B^{ij}(x) \frac{\partial \Phi(x)}{\partial x^j} = 0 \tag{5b}$$

Thus $\partial \Phi / \partial x^j$ must be a null vector of B^{ij} at each point x. From this equation follows, on differentiating with respect to x^i

$$\frac{\partial B^{ij}}{\partial x^i} \frac{\partial \Phi}{\partial x^j} + B^{ij} \frac{\partial^2 \Phi}{\partial x^i \, \partial x^j} = 0$$

Hence, the second of the conditions (5) may be written

$$\left\{ A^i - \frac{1}{2} \frac{\partial B^{ij}}{\partial x^j} \right\} \frac{\partial \Phi}{\partial x^i} = 0 \tag{6}$$

Remark. The conditions may be interpreted in the following way. Write (3) as a continuity equation for the probability density, involving a flux J^i

$$\frac{\partial P}{\partial t} = -\frac{\partial J^i}{\partial x^i}, \qquad J^i = \left(A^i - \frac{1}{2} \frac{\partial B^{ij}}{\partial x^j} \right) P - \frac{1}{2} B^{ij} \frac{\partial P}{\partial x^j} \tag{7}$$

The two terms of J^i are proportional to P and to its gradient and may therefore be considered as the convective and diffusive flows, respectively. The fact that Φ is conserved is expressed by

$$J^i \frac{\partial \Phi}{\partial x_i} = 0$$

Equations (5b) and (6) state that Φ must be conserved by the convective and diffusive flows separately.

It must be remarked, however, that under the transformation

$$\frac{\partial \bar{P}}{\partial t} = -\frac{\partial \bar{J}^k}{\partial \bar{x}^k}, \qquad \bar{J}^k = \left(J^i \frac{\partial \bar{x}^k}{\partial x^i} \right) \left| \text{Det} \frac{\partial \bar{x}^k}{\partial x^i} \right|^{-1}$$

the two terms of $\bar{J}^k$ do not correspond separately to those of J^i (unless the transformation determinant is constant). Hence, the separation in convective and diffusive flows is not invariant for coordinate transformations, although of course both conditions (5) together are.

Suppose (3) has n functionally independent conserved quantities $\Phi^\nu(x)$. Choose as new variables $\bar{x}^k$ the quantities

$$z^\nu = \Phi^\nu(x) \qquad (\nu = 1, 2, \ldots, n)$$

together with $d - n$ supplementary functions $y^r(x)$. Then the submanifold $\mathbb{M}$ is determined by

$$z^\nu \equiv \Phi^\nu(x) = c^\nu \qquad (\nu = 1, 2, \ldots, n) \tag{8}$$

and the y^r are coordinates on $\mathbb{M}$. In order that the transformation is invertible one must require that the gradients $\partial \Phi^\nu / \partial x^i$ of the Φ^ν are linearly independent, at least on $\mathbb{M}$.

In these new variables the fact that the z^ν are conserved implies, according to (5)

$$\bar{B}^{k\nu} = 0, \qquad \bar{A}^\nu = 0$$

Hence the transformed equation is

$$\frac{\partial \bar{P}(y, z, t)}{\partial t} = -\frac{\partial}{\partial y^r} \bar{A}^r(y, z) \, \bar{P} + \frac{1}{2} \frac{\partial^2}{\partial y^r \, \partial y^s} \bar{B}^{rs}(y, z) \, \bar{P}$$

As no differentiations with respect to the z^ν occur there are solutions of the form

$$\bar{P}(y, z, t) = S(y) \prod_\nu \delta(z^\nu - c^\nu)$$

Their support is $\mathbb{M}$. The surface density S obeys a Smoluchowski equation with $d-n$ variables

$$\frac{\partial S(y,t)}{\partial t} = -\frac{\partial}{\partial y^r}\bar{A}^r(y,c)\,S + \frac{1}{2}\frac{\partial^2}{\partial y^r\,\partial y^s}\bar{B}^{rs}(y,c)\,S$$

Summary

For the Fokker–Planck equation (3) each conserved quantity constitutes a mathematical constraint and enables one to eliminate one variable. There remains a reduced Fokker–Planck equation on the manifold determined by (8).

3. A PHYSICAL CONSTRAINT

Consider two-dimensional diffusion in an inhomogeneous, anisotropic medium and a field of force, as described by (3) with positive definite B^{ij}. Let the diffusing particle be confined to a narrow strip in the plane, lying between two curves given by

$$\Phi(x^1, x^2) = 0 \qquad \text{and} \qquad \Phi(x^1, x^2) = \varepsilon \tag{9}$$

At these boundaries the particle is reflected so that the normal component of the probability flow (7) vanishes

$$\frac{\partial \Phi}{\partial x^i}\left(A^i P - \frac{1}{2}\frac{\partial}{\partial x^j} B^{ij} P\right) = 0 \qquad (\Phi = 0, \varepsilon) \tag{10}$$

Transform to the new variable $z = \Phi(x^1, x^2)$ and an arbitrary supplementary variable $y(x^1, x^2)$, which serves as a coordinate along the strip. The diffusion equation transforms into

$$\frac{\partial \bar{P}(y,z,t)}{\partial t} = -\frac{\partial}{\partial y}\bar{A}^y\bar{P} + \frac{1}{2}\frac{\partial^2}{\partial y^2}\bar{B}^{yy}\bar{P} + \frac{\partial}{\partial z}\left[-\bar{A}^z\bar{P} + \frac{\partial}{\partial y}\bar{B}^{zy}\bar{P} + \frac{1}{2}\frac{\partial}{\partial z}\bar{B}^{zz}\bar{P}\right] \tag{11}$$

The boundary condition (10) is invariant under the transformation and therefore becomes

$$\bar{A}^z\bar{P} - \frac{1}{2}\frac{\partial}{\partial y}\bar{B}^{zy}\bar{P} - \frac{1}{2}\frac{\partial}{\partial z}\bar{B}^{zz}\bar{P} = 0 \qquad (z = 0, \varepsilon) \tag{12}$$

Physically one might expect that $\bar{P}$ becomes constant across the strip, but this boundary condition shows that that is not possible. We have to proceed more carefully.

We take the average of the density across the strip as the "surface density" on the curve $\Phi = 0$

$$S(y, t) = \frac{1}{\varepsilon} \int_0^\varepsilon P(y, z, t)\, dz \tag{13}$$

Integrating (11) across the strip one obtains

$$\begin{aligned} \frac{\partial S(y, t)}{\partial t} = &-\frac{\partial}{\partial y} \bar{A}^y(y, 0)\, S + \frac{1}{2} \frac{\partial^2}{\partial y^2} \bar{B}^{yy}(y, 0)\, S \\ &+ \frac{1}{\varepsilon} \left[-\bar{A}^z \bar{P} + \frac{\partial}{\partial y} \bar{B}^{zy} \bar{P} + \frac{1}{2} \frac{\partial}{\partial z} \bar{B}^{zz} \bar{P} \right]_{z=0}^{z=\varepsilon} \end{aligned} \tag{14}$$

On the first line the coefficients $\bar{A}^y(y, z)$ and $\bar{B}^{zz}(y, z)$ have been identified with their values on the manifold $z = 0$, neglecting terms of order ε. The integrated term on the second line is not quite the same as that which occurs in the boundary condition (12), and therefore a remnant of it survives

$$\frac{1}{2\varepsilon} \frac{\partial}{\partial y} [\bar{B}^{zy}(y, z)\, \bar{P}(y, z, t)]_{z=0}^{z=\varepsilon}$$

As a consequence (14) is *not* a self-contained diffusion equation for $S(y, t)$, unless $\bar{B}^{zy} = 0$.

In order to achieve this, one must choose $y(x^1, x^2)$ so as to obey the linear first-order partial differential equation

$$\bar{B}^{zy} \equiv \frac{\partial \Phi}{\partial x^i} B^{ij}(x) \frac{\partial y}{\partial x^j} = 0 \tag{15}$$

The equation states that the curves of constant y are orthogonal to those of constant z with respect to the metric given by B^{ij}. It can be solved, and since B^{ij} is positive-definite the family of curves is unique. Hence, the function $y(x^1, x^2)$ is unique up to an arbitrary transformation of the form $y = \chi(y')$.

The conclusion is that diffusion in two dimensions with one physical constraint (9) can be reduced in the limit $\varepsilon \to 0$ to a diffusion equation on $\mathbb{M}$:

$$\frac{\partial S(y, t)}{\partial t} = -\frac{\partial}{\partial y} \bar{A}^y(y)\, S + \frac{1}{2} \frac{\partial^2}{\partial y^2} \bar{B}^{yy}(y)\, S \tag{16}$$

where y is any arbitrary parameter along the curve $\Phi = 0$ and $S(y, t)\, dy$ the probability for finding the particle between y and $y + dy$.

This result, however, depends crucially on (15), which in this simple case always has a solution. In general, however, one has a d-dimensional space $\mathbb{R}^d$ in which a $(d-n)$-dimensional manifold $\mathbb{M}$ is embedded given by (8). The physical constraint is represented by a tubular space around $\mathbb{M}$

$$c^\nu < \Phi^\nu(x) < c^\nu + \varepsilon \tag{17}$$

Inside this tubular space, diffusion takes place described by (3), with reflection on the boundary.

Instead of the functions Φ^ν one may use for specifying $\mathbb{M}$ any set of functions

$$\Psi^\mu(x) = h^\mu_\nu(x)\, \Phi^\nu(x)$$

where the $h^\mu_\nu(x)$ are arbitrary functions whose determinant does not vanish. The corresponding tubular space

$$c^\nu < \Psi^\nu(x) < c^\nu + \varepsilon$$

is not the same as (17). Accordingly we formulate our problem: Is it possible to choose functions $y^r(x)$, $z^\nu(x)$ such that: (i) the given manifold $\mathbb{M}$ corresponds with $z^\nu = 0$, and (ii)

$$\bar{B}^{\nu r} \equiv \frac{\partial z^\nu}{\partial x^i} B^{ij}(x) \frac{\partial y^r}{\partial x^j} = 0 \qquad \text{(all } \nu, r) \tag{18}$$

This is, in analogy with (15), the condition that in the limit $\varepsilon \to 0$ the diffusion in the tubular space obeys an autonomous equation on $\mathbb{M}$. Without loss of generality we took $c^\nu = 0$. As can be seen from (14) it suffices that (18) holds to order $|z|^2$.

The problem formulated in this way is a question of differential geometry and is treated in the Appendix. The upshot is that it is *not* true that for all $\mathbb{M} \subset \mathbb{R}^d$ such a set of variables exists. Hence *it is not true that for any given manifold one can find a physical constraint which in the limit* $\varepsilon \to 0$ *leads to an autonomous diffusion equation on that manifold.* The exceptions, however, do not occur in two or three dimensions. Admittedly only constraints of the type (17) have been allowed, but I expect the result to be general.

4. THE KRAMERS EQUATION

Three different descriptions of Brownian motion exist. In the first one, due to Einstein and Smoluchowski,[11] the x^i were the coordinates $\mathbf{r}_n$ of the particles. We call this the Smoluchowski case; it was the subject of the preceding section. In the description by Rayleigh[12] and Langevin,[13,14] the x^i stand for the velocities $\mathbf{r}_n$. It applies to a finer time scale, on which the inertia of the Brownian particle cannot be neglected. But it is restricted to spatial homogeneity. It has been called after Rayleigh.[15]

We are concerned with the third case, called after Kramers,[16] which combines the two previous ones. One half of the x^i stand for the coordinates and the other half for their velocities, or functions thereof, e.g., the momenta. For the two sets of variables we write x^α and u^α. Thus our phase space is the tangent bundle of the configuration space of the x^α. The Fokker–Planck equation takes the form

$$\frac{\partial P(x, u, t)}{\partial t} = -\frac{\partial}{\partial x^\alpha} G^\alpha(x, u)\, P - \frac{\partial}{\partial u^\alpha} A^\alpha(x, u)\, P + \frac{1}{2} \frac{\partial^2}{\partial u^\alpha\, \partial u^\beta} B^{\alpha\beta}(x, u)\, P \tag{19}$$

It is of the general form (3) with

$$A^i = (G^\alpha, A^\alpha), \qquad B^{ij} = \begin{pmatrix} 0 & 0 \\ 0 & B^{\alpha\beta} \end{pmatrix}$$

The zeros appearing in the block matrix B express the fact that the random forces act only on the velocities.

In the Kramers case it is natural to consider only point transformations, i.e., the subgroup of (4) determined by

$$\bar{x}^\alpha = \varphi^\alpha(x), \qquad \bar{u}^\alpha = \psi^\alpha(x, u) \tag{20}$$

because they preserve the form of (19). The general formula (4) yields

$$\bar{P}(\bar{x}, \bar{u}, \bar{t}) = P(x, u, t) \left| \left(\mathrm{Det}\, \frac{\partial \varphi^\alpha}{\partial x^\beta} \right) \left(\mathrm{Det}\, \frac{\partial \psi^\alpha}{\partial u^\beta} \right) \right|^{-1} \tag{21a}$$

$$\bar{G}^\alpha = G^\beta \frac{\partial \varphi^\alpha}{\partial x^\beta}, \qquad \bar{B}^{\alpha\beta} = B^{\gamma\delta} \frac{\partial \psi^\alpha}{\partial u^\gamma} \frac{\partial \psi^\beta}{\partial u^\delta} \tag{21b}$$

$$\bar{A}^\alpha = A^\beta \frac{\partial \psi^\alpha}{\partial u^\beta} + G^\beta \frac{\partial \psi^\alpha}{\partial x^\beta} + \frac{1}{2} B^{\gamma\delta} \frac{\partial^2 \psi^\alpha}{\partial u^\gamma\, \partial u^\delta} \tag{21c}$$

If the u^α are the velocities themselves, $G^\alpha(x, u) = u^\alpha$, then (19) reduces to the specific form given by Klein[17] and Kramers[16]

$$\frac{\partial P(x, u, t)}{\partial t} = -u^\alpha \frac{\partial P}{\partial x^\alpha} - \frac{\partial}{\partial u^\alpha} A^\alpha P + \frac{1}{2} \frac{\partial^2}{\partial u^\alpha\, \partial u^\beta} B^{\alpha\beta} P \tag{22}$$

This form is preserved by the transformations

$$\bar{x}^\alpha = \varphi^\alpha(x), \qquad \bar{u}^\alpha = \frac{\partial \varphi^\alpha(x)}{\partial x^\beta} u^\beta \tag{23}$$

One finds

$$\bar{P}(\bar{x}, \bar{u}, \bar{t}) = P(x, u, t) \left| \mathrm{Det} \frac{\partial \varphi^\alpha}{\partial x^\beta} \right|^{-2} \tag{24a}$$

$$\bar{A}^\alpha = A^\beta \frac{\partial \varphi^\alpha}{\partial x^\beta} + u^\beta u^\gamma \frac{\partial^2 \varphi^\alpha}{\partial x^\beta \partial x^\gamma} \tag{24b}$$

$$\bar{B}^{\alpha\beta} = B^{\gamma\delta} \frac{\partial \varphi^\alpha}{\partial x^\gamma} \frac{\partial \varphi^\beta}{\partial x^\delta} \tag{24c}$$

Remark. These transformation equations may be expressed in familiar symbols of differential geometry, viz.

$$g_{\alpha\beta} = \frac{\partial x^\gamma}{\partial \bar{x}^\alpha} \frac{\partial x^\gamma}{\partial \bar{x}^\beta}, \qquad g_{\alpha\beta} g^{\beta\gamma} = \delta^\gamma_\alpha, \tag{25a}$$

$$\Gamma^\gamma_{\alpha\beta} = \frac{1}{2} g^{\gamma\delta} \left(\frac{\partial g_{\alpha\delta}}{\partial \bar{x}^\beta} + \frac{\partial g_{\beta\delta}}{\partial \bar{x}^\alpha} - \frac{\partial g_{\alpha\beta}}{\partial \bar{x}^\delta} \right) \tag{25b}$$

The transform of (22) can be written[9]

$$\frac{\partial \bar{P}}{\partial t} = -\bar{u}^\alpha \frac{\partial \bar{P}}{\partial \bar{x}^\alpha} + \frac{\partial}{\partial \bar{u}^\gamma} \Gamma^\gamma_{\alpha\beta} \bar{u}^\alpha \bar{u}^\beta \bar{P} - \frac{\partial}{\partial \bar{u}^\alpha} \tilde{A}^\alpha \bar{P} + \frac{1}{2} \frac{\partial^2}{\partial \bar{u}^\alpha \partial \bar{u}^\beta} \bar{B}^{\alpha\beta} \bar{P} \tag{26}$$

where

$$\tilde{A}^\alpha = A^\beta \frac{\partial \varphi^\alpha}{\partial x^\beta}$$

is a covariant vector, while $\bar{B}^{\alpha\beta}$ is a covariant tensor according to (24c).

The condition that $\Phi(x, u)$ is a conserved quantity of (19) takes the form

$$B^{\alpha\beta} \frac{\partial \Phi}{\partial u^\beta} = 0, \qquad G^\alpha \frac{\partial \Phi}{\partial x^\alpha} = 0, \qquad \left(A^\alpha - \frac{1}{2} \frac{\partial B^{\alpha\beta}}{\partial u^\beta} \right) \frac{\partial \Phi}{\partial u^\alpha} = 0 \tag{27}$$

If Φ is a function of the x^α alone, not involving the u^α, one may apply a transformation (23) such that $\bar{x}^1 = \Phi(x)$. Then $\bar{G}^1 = 0$, so that the transformed equation contains no differentiation with respect to x^1, and x^1 only enters as a parameter in the coefficients. If, on the other hand, Φ does involves the u^α, one may use (20) with $\bar{u}^1 = \Phi(x, u)$ and, as a result, $\bar{B}^{\alpha 1} = 0$ and $\bar{A}^1 = 0$, so that $\bar{u}^1$ is reduced to a parameter. In this way a mathematical constraint has again been used to decrease the number of variables in (19).

In the Kramers equation (22) a conserved quantity is, according to (27), necessarily a function of u alone. A function $\Phi(u)$, however, cannot in general be utilized as a new velocity $\bar{u}^1$ unless it is linear, as required by (23). Otherwise, one has to use the more general transformation (20) and the transformed equation will have the general form (19) rather than (22).

Remark. The Kramers case resembles classical mechanics in that both coordinates and velocities enter, but it should be compared with mechanical systems with damping rather than with Lagrange mechanics. In the latter case a constant of the motion $\Phi(x) = c$ allows one to eliminate one degree of freedom, i.e., one variable q_1 together with its velocity $\dot{q}_1$. We, however, have merely been able to eliminate one coordinate $\bar{x}^1$ but all $\bar{u}^\alpha$ are still present.

Yet in a special case one can eliminate $\bar{u}^1$ as well. Suppose that in the transformed equation all coefficients $\bar{A}^\alpha$, $\bar{B}^{\alpha\beta}$ with $\alpha, \beta \neq 1$ are independent of $\bar{u}^1$. It is then possible to integrate the equation over $\bar{u}^1$ so as to obtain a closed equation for

$$\int_{-\infty}^{\infty} P(x, y, t)\, du^1 = S(x^2, x^3, \ldots, u^2, u^3, \ldots, t) \tag{28}$$

Only in this case does one really have a Kramers equation on the tangent bundle of $\mathbb{M}$.

5. LIGHT RAYS IN RANDOM MEDIUM AS EXAMPLE OF A KRAMERS EQUATION WITH MATHEMATICAL CONSTRAINT

Our first task is to establish an appropriate description in terms of a Fokker–Planck equation. A light ray in an inhomogeneous medium with refractive index $n(x)$ obeys[18]

$$\frac{dx^\alpha}{ds} = u^\alpha, \qquad \frac{du^\alpha}{ds} = (\delta^{\alpha\beta} - u^\alpha u^\beta)\frac{\partial \log n}{\partial x^\beta} \tag{29}$$

s is the arc length along the ray, the superscripts refer to the coordinates x, y, z in space, and u^α is the tangent unit vector

$$u^\alpha u_\alpha = 1 \qquad (u_\alpha = u^\alpha) \tag{30}$$

This is a mathematical constraint of type (2). The Liouville equation equivalent with (29) is

$$\frac{\partial\rho(x,u,t)}{\partial t}=-u^{\alpha}\frac{\partial\rho}{\partial x^{\alpha}}-\frac{\partial}{\partial u^{\alpha}}\Delta^{\alpha\beta}\frac{\partial\log n}{\partial x^{\beta}}\rho \tag{31}$$

where $\Delta^{\alpha\beta}=\delta^{\alpha\beta}-u^{\alpha}u^{\beta}$.

Suppose $n(x)$ has a small random component; we may set

$$\log n(x)=\mu(x)+\varepsilon\kappa(x),\qquad \langle\kappa(x)\rangle=0$$

Then (31) is a linear stochastic differential equation of the form

$$\frac{\partial\rho}{\partial s}=(L+\varepsilon K)\,\rho$$

$$L=-u^{\alpha}\frac{\partial}{\partial x^{\alpha}}-\frac{\partial}{\partial u^{\alpha}}\Delta^{\alpha\beta}\mu_{,\beta},\qquad K=-\frac{\partial}{\partial u^{\alpha}}\Delta^{\alpha\beta}\kappa_{,\beta}$$

The differential operators act on everything to the right while $\mu_{,\beta}$, $\kappa_{,\beta}$ are derivatives with respect to x^{β}. To second order in ε one obtains for the probability density $P(x,u,t)=\langle\rho(x,u,t)\rangle$ the Fokker–Planck equation[19]

$$\begin{aligned}\frac{\partial P}{\partial s}&=\left[L+\varepsilon^{2}\int_{0}^{\infty}\langle Ke^{\sigma L}K\rangle\,e^{-\sigma L}\,d\sigma\right]P\\&=-u^{\alpha}\frac{\partial P}{\partial x^{\alpha}}-\frac{\partial}{\partial u^{\alpha}}\Delta^{\alpha\beta}\mu_{,\beta}P\\&\quad+\varepsilon^{2}\frac{\partial}{\partial u^{\alpha}}\int_{0}^{\infty}d\sigma\,\Delta^{\alpha\beta}\left\langle\kappa_{,\beta}\left[\frac{\partial}{\partial u^{\gamma}}\Delta^{\gamma\delta}\kappa_{,\delta}\right]_{-\sigma}\right\rangle P\end{aligned}\tag{32}$$

This approximation holds when $\varepsilon\xi\ll 1$, where ξ is the autocorrelation length of $\kappa(x)$:

$$\langle\kappa(x)\,\kappa(x')\rangle\approx 0\qquad\text{for}\qquad |x-x'|>\xi$$

The subscript $-\sigma$ indicates that one has to insert the values of x, u at a distance σ back along the ray. If μ is constant, or if

$$\xi\,|\nabla\mu|\ll 1 \tag{33}$$

one may take

$$[x^{\alpha}]_{-\sigma}=x^{\alpha}-\sigma u^{\alpha},\qquad [u^{\alpha}]_{-\sigma}=u^{\alpha}$$

so that

$$\left[\frac{\partial}{\partial u^\gamma} \Delta^{\gamma\delta} \kappa_{,\delta}\right]_{-\sigma} = \left(\frac{\partial}{\partial u^\gamma} + \sigma \frac{\partial}{\partial x^\gamma}\right) \Delta^{\gamma\delta}(u)\, \kappa_{,\delta}(x - \sigma u)$$

Hence, the last term of (32) becomes

$$\varepsilon^2 \frac{\partial}{\partial u^\alpha} \Delta^{\alpha\beta} \int_0^\infty d\sigma \langle \kappa_{,\beta}(x)\, \kappa_{,\delta}(x - \sigma u)\rangle \left(\frac{\partial}{\partial u^\gamma} + \sigma \frac{\partial}{\partial x^\gamma}\right) \Delta^{\gamma\delta} P$$

The term containing σ as a factor is one order of ξ higher than the other and will be neglected. Also we abbreviate

$$\int_0^\infty d\sigma \langle \kappa_{,\beta}(x)\, \kappa_{,\delta}(x - \sigma u)\rangle = C_{\beta\delta}(x, u)$$

and obtain

$$\varepsilon^2 \frac{\partial^2}{\partial u^\alpha\, \partial u^\gamma} \Delta^{\alpha\beta} \Delta^{\gamma\delta} C_{\beta\delta} P - \varepsilon^2 \frac{\partial}{\partial u^\alpha} \Delta^{\gamma\delta} \left(\frac{\partial}{\partial u^\gamma} \Delta^{\alpha\beta} C_{\beta\delta}\right) P$$

Thus our Fokker–Planck equation (32) takes the form of the Kramers equation (22) with

$$B^{\alpha\beta} = 2\varepsilon^2 \Delta^{\alpha\gamma} \Delta^{\beta\delta} C_{\gamma\delta}$$

$$A^\alpha = \Delta^{\alpha\beta} \mu_{,\beta} + \varepsilon^2 \Delta^{\beta\delta} \left(\frac{\partial}{\partial u^\beta} \Delta^{\alpha\gamma} C_{\gamma\delta}\right)$$

Having established the equation we first notice that it is compatible with the constraint (30) because (27) is satisfied, as is easily verified. Hence it is permissible to transform to new variables θ, φ by setting

$$u_x = \sin\theta \cos\varphi, \qquad u_y = \sin\theta \sin\varphi, \qquad u_z = \cos\theta$$

The explicit computation is somewhat simplified if we assume the fluctuations $\kappa(x)$ to be isotropic, so that $C_{\gamma\delta}(x, u)$ must be a tensor:

$$C_{\gamma\delta}(x, u) = \delta_{\gamma\delta} C_0(x) + u_\gamma u_\delta C_1(x), \qquad \Delta^{\alpha\gamma} C_{\gamma\delta} = C_0\, \Delta^\alpha_\delta = C_0\, \Delta^{\alpha\delta}$$

$$B^{\alpha\beta} = 2\varepsilon^2 C_0\, \Delta^{\alpha\beta}, \qquad A^\alpha = \Delta^{\alpha\beta} \mu_{,\beta} - 2\varepsilon^2 C_0 u^\alpha$$

Explicit computation with the aid of (4b) gives

$$\frac{\partial \bar{P}(x, y, z, \theta, \varphi, s)}{\partial s}$$

$$= -\sin\theta\cos\varphi\frac{\partial \bar{P}}{\partial x} - \sin\theta\sin\varphi\frac{\partial \bar{P}}{\partial y} - \cos\theta\frac{\partial \bar{P}}{\partial z}$$

$$-\frac{\partial}{\partial\theta}\left[\mu_{,x}\cos\theta\cos\varphi + \mu_{,y}\cos\theta\sin\varphi - \mu_{,z}\sin\theta + \varepsilon^2 C_0\cot\theta\right]\bar{P}$$

$$-\frac{\partial}{\partial\varphi}\left[\frac{\mu_{,x}\sin\varphi + \mu_{,y}\cos\varphi}{\sin\theta}\right]\bar{P} + \varepsilon^2 C_0\left(\frac{\partial^2 \bar{P}}{\partial\theta^2} + \frac{1}{\sin^2\theta}\frac{\partial^2 \bar{P}}{\partial\varphi^2}\right)$$

In a homogeneous medium μ and C_0 are constant. Then a number of terms vanish and the remaining equation can be integrated over space. One is then left with a Rayleigh equation for the probability distribution of the direction alone

$$\frac{\partial P(\theta, \varphi, s)}{\partial s} = \varepsilon^2 C_0\left\{-\frac{\partial}{\partial\theta}\cot\theta\, P + \frac{\partial^2 P}{\partial\theta^2} + \frac{1}{\sin^2\theta}\frac{\partial^2 P}{\partial\varphi^2}\right\}$$

Its stationary solution is $P = \sin\theta$, which is the expected constant density on the unit sphere.

6. THE KRAMERS EQUATION WITH A PHYSICAL CONSTRAINT

Our model is two-dimensional Brownian motion described by the Kramers equation (22) and confined to the same strip as in Section 3. At the two boundary curves (9) the particle is specularly reflected. This is expressed by

$$P(x, u, t) = P(x, u^*, t) \qquad (x \text{ on boundary})$$

where u^* denotes the velocity u with reversed normal component.

We transform again to the variables $z = \Phi(x^1, x^2)$ and $y(x^1, x^2)$ but now require the coordinates y to be orthogonal to the z (which in two dimensions can be achieved). The two velocities transform according to (23) into

$$w = \frac{\partial\Phi}{\partial x^\beta}u^\beta, \qquad v = \frac{\partial y}{\partial x^\beta}u^\beta$$

The transformed equation is given by (24) or (26) and the boundary condition is, thanks to the orthogonality,

$$\bar{P}(y, z, v, w, t) = \bar{P}(y, z, v, -w, t) \qquad \text{for} \qquad z = 0, \varepsilon \tag{34}$$

Our aim is not just to eliminate z, but also w, so as to obtain a Kramers equation for the motion on the curve $\mathbb{M}$ alone. Hence it is not sufficient to integrate across the strip as in the Smoluchowski case in Section 3.

When we set $z = \varepsilon\zeta$ the transformed equation may be written in the form (26)

$$\frac{\partial \bar{P}(y, z, v, w, t)}{\partial t} = \left[\frac{1}{\varepsilon}\mathscr{L}^{(0)} + \mathscr{L}^{(1)}\right]\bar{P} \tag{35}$$

$$\mathscr{L}^{(0)} = -w\frac{\partial}{\partial \zeta}$$

$$\begin{aligned}\mathscr{L}^{(1)} = {} & -v\frac{\partial}{\partial y} + \frac{\partial}{\partial v}(\Gamma^1_{11}v^2 + 2\Gamma^1_{12}vw + \Gamma^1_{22}w^2)\,\bar{P} \\ & + \frac{\partial}{\partial w}(\Gamma^2_{11}v^2 + 2\Gamma^2_{12}vw + \Gamma^2_{22}w^2)\,\bar{P} - \frac{\partial}{\partial v}\tilde{A}^1\bar{P} - \frac{\partial}{\partial w}\tilde{A}^2\bar{P} \\ & + \frac{1}{2}\frac{\partial^2}{\partial v^2}\bar{B}^{11}\bar{P} + \frac{\partial^2}{\partial v\,\partial w}\bar{B}^{12}\bar{P} + \frac{1}{2}\frac{\partial^2}{\partial w^2}\bar{B}^{22}\bar{P}\end{aligned}$$

Taking into account that the coordinates $\bar{x}^1 = y$, $\bar{x}^2 = z$ are orthogonal, one finds from (25)

$$\Gamma^1_{11} = \frac{1}{2}\frac{\partial \log g_{yy}}{\partial y} \qquad \Gamma^1_{21} = \frac{1}{2}\frac{\partial \log g_{yy}}{\partial z}$$

$$\Gamma^1_{22} = -\frac{1}{2g_{yy}}\frac{\partial g_{zz}}{\partial y} \qquad \Gamma^2_{11} = -\frac{1}{2g_{zz}}\frac{\partial g_{yy}}{\partial z}$$

$$\Gamma^2_{12} = \frac{1}{2}\frac{\partial \log g_{zz}}{\partial y} \qquad \Gamma^2_{22} = \frac{1}{2}\frac{\partial \log g_{zz}}{\partial z}$$

We are interested in those solutions of (35) that tend to a limit as ε goes to zero. They can be found by means of the general method developed for eliminating fast variables.[20] First one has to use the left null vectors of $\mathscr{L}^{(0)}$ for the construction of a projection operator $\mathscr{P}$ having the property $\mathscr{P}\mathscr{L}^{(0)} = 0$. Explicitly

$$\mathscr{P}\mathscr{L}^{(0)}p(y, \zeta, v, w) \equiv -\mathscr{P}w\frac{\partial p}{\partial \zeta} = 0$$

for all functions p obeying the boundary condition (34). This requirement is fulfilled by taking

$$\mathscr{P}p(y, \zeta, v, w) = \frac{1}{2}\int_0^1 \{p(y, \zeta, v, w) + p(y, \zeta, v, -w)\}\, d\zeta$$

Evidently it happens that also $\mathscr{L}^{(0)}\mathscr{P} = 0$. As a result, one has for the projected function $\mathscr{P}\bar{P} = R$ in the limit $\varepsilon \to 0$[20,21]

$$\begin{aligned}\frac{\partial R(y, v, w, t)}{\partial t} &= (\mathscr{P}\mathscr{L}^{(1)}\mathscr{P})\, R \\ &= -v\frac{\partial R}{\partial y} + \frac{\partial}{\partial v}(\Gamma^1_{11} v^2 + \Gamma^1_{22} w^2)\, R \\ &\quad + 2\Gamma^2_{12} v \frac{\partial}{\partial w} wR - \frac{\partial}{\partial v}\overset{\mathrm{e}}{\tilde{A}}{}^1 R - \frac{\partial}{\partial w}\overset{\mathrm{o}}{\tilde{A}}{}^2 R \\ &\quad + \frac{1}{2}\frac{\partial^2}{\partial v^2}\overset{\mathrm{e}}{\bar{B}}{}^{11} R + \frac{\partial^2}{\partial v\, \partial w}\overset{\mathrm{o}}{\bar{B}}{}^{12} R + \frac{1}{2}\frac{\partial^2}{\partial w^2}\overset{\mathrm{e}}{\bar{B}}{}^{22} R \end{aligned} \tag{36}$$

The superposed e and o indicate the even and odd parts of $\tilde{A}^\alpha$ and $\bar{B}^{\alpha\beta}$ as functions of w. In all coefficients the variable z is to be set to zero.

Thus the physical constraint has enabled us to eliminate the variable z, but not yet w. We merely know that R must be an even function of w. The distribution of y, v alone is

$$S(y, v, t) = \int_{-\infty}^{\infty} R(y, v, w, t)\, dw$$

On integrating (36), however, one obtains

$$\begin{aligned}\frac{\partial S(y, v, t)}{\partial t} &= -v\frac{\partial S}{\partial y} + \Gamma^1_{22}\frac{\partial}{\partial v} v^2 S \\ &\quad + \Gamma^1_{22}\frac{\partial}{\partial v}\int w^2 R\, dw - \frac{\partial}{\partial v}\int \tilde{A}^1 R\, dw \\ &\quad + \frac{1}{2}\frac{\partial^2}{\partial v^2}\int \bar{B}^{11} R\, dw \end{aligned} \tag{37}$$

What are the conditions for it to become a closed equation for S?

The last term can be expressed in S alone if $\bar{B}^{11}$ is independent of w. (This is certainly the case if we are dealing with ordinary Brownian motion, since in that case $B^{\alpha\beta}$ is independent of all vectories.) The next but last term in (37) requires $\tilde{A}^1$ to be independent of w (which is true for Brownian motion if the medium is isotropic).

The first term on the second line of (37), however, involves the mean square of the transverse velocity and cannot be expressed in S alone for any type of Brownian motion. It is harmless only if $\Gamma^1_{22} = 0$ that is, if

$$0 = \frac{\partial g_{22}}{\partial y} = \frac{\partial}{\partial y}\left(\frac{\partial x^i}{\partial z}\right)^2$$

It means that the spatial distance between the points $z = 0$ and $z = \varepsilon$ must not vary along the strip: the strip must have a constant width. Thus *only if the strip has a constant width does one obtain an autonomous equation for the surface density* $S(y, v, t)$. (We ignore the one remaining possibility, namely

$$\Gamma^1_{22} w^2 - \tilde{A}^1 = 0$$

because it does not appear to have any physical implementation.)

If this condition is not satisfied, the term with Γ^1_{22} in (37) survives and the dependence of R on w cannot be eliminated. The integral is the transverse component of the pressure tensor and the whole term describes how this transverse pressure pushes the particle toward wider parts of the strip. Of course no such effect exists in the Smoluchowski case.

7. BROWNIAN ROTATION AS AN EXAMPLE OF THE HEURISTIC APPROACH

So far our physical constraints consisted of reflecting walls. The Brownian particle could also be constrained to move on a manifold by a potential that sharply rises away from $\mathbb{M}$, say $\varepsilon^{-1} W(x)$, where

$$W(x) = \frac{1}{2} \sum_{\nu} [\Phi^{\nu}(x)]^2$$

More generally, one could take as constraining potential

$$W(x) = \tfrac{1}{2} l_{\nu\mu}(x)\, \Phi^{\nu}(x)\, \Phi^{\mu}(x) \tag{38}$$

with a positive definite matrix of functions $l_{\nu\mu}$. This is the type of constraint that is implicit in Lagrange mechanics.[4] Hence, if one has a mechanical system that is confined to a manifold $\mathbb{M}$ by Lagrangian constraints and is subject to random forces, one must confine the motion by (38) rather than by reflecting walls. The correct choice of W is determined by the actual constraining force.

More precisely, one should start from the Newton equations including the potential $\varepsilon^{-1}W$, then add the fluctuating forces (and of course also damping), and *finally* take the limit $\varepsilon \to 0$. However, this is not what is normally done. Instead one starts from the Lagrange equations, which is the same as Newton mechanics with $\varepsilon^{-1}W$ in the limit $\varepsilon \to 0$, and only *after having taken this limit* one adds fluctuations. The proper form of the fluctuation terms is then somewhat of a guess, since the connection with the actual fluctuating forces is lost. The result is by construction a Fokker–Planck equation on the fiber bundle of a manifold, but its physical validity is not ascertained.

Nonetheless we now apply this doubtful approach to the Brownian rotation of a rigid body. The purpose is to demonstrate how the terms describing fluctuations and damping are guessed and to obtain a Fokker–Planck equation on a manifold, which in the future may be compared to the result of a correct calculation.

Classical mechanics treats a rigid body as a collection of point masses m_n with a large number of constraints that have the effect of fixing all mutual distances. The coordinates of the masses in space may be written

$$\mathbf{r}_n = \mathbf{R} + O(q)\,\mathbf{r}_n^*$$

where $\mathbf{R}$ is the center of mass, $\mathbf{r}_n^*$ the coordinates with respect to axes fixed in the body, and $O(q)$ a three-dimensional orthogonal matrix, parametrized by three variables q^α, for instance the Eulerian angles. For simplicity we also impose the constraint $\mathbf{R}=0$ so that we are left with the three Lagrange variables q^α. The manifold $\mathbb{M}$ is the group manifold of O(3). The kinetic energy is

$$\frac{1}{2}\sum_n m_n \mathbf{r}_n^* \cdot \frac{\partial O^+}{\partial q^r}\frac{\partial O}{\partial q^s}\cdot \mathbf{r}_n \dot{q}^r \dot{q}^s = \frac{1}{2} k_{rs}(q)\,\dot{q}^r\dot{q}^s$$

In the presence of a potential $U(q)$ one obtains for the velocities $\dot{q}^r = u^r$ the equations of motion

$$\dot{u}^r = -G^r_{ij}(q)\,u^i u^j - k^{rs}(q)\frac{\partial U}{\partial q^s}$$

where k^{rs} is the reciprocal of k_{rs} and G^r_{ij} are the Christoffel symbols (25) constructed from the k_{rs}.

In order to introduce damping one adds an *ad hoc* friction term $-f^r_s u^s$, where the coefficients f^r_s may depend on q and u. This deterministic system has a Liouville equation for the density in the phase space of q and u. To introduce fluctuations one adds to this equation a term with second-order derivatives[16,22,9] so as to obtain the Fokker–Planck equation

$$\frac{\partial P(q, u, t)}{\partial t} = -u^r \frac{\partial P}{\partial q^r} + \frac{\partial}{\partial u^r}\left(G^r_{ij} u^i u^j + k^{rs} \frac{\partial U}{\partial q^s}\right) P$$
$$+ \frac{\partial}{\partial u^r}\left(f^r_s u^s + \frac{1}{2}\frac{\partial}{\partial u^s} B^{rs}\right) P \tag{39}$$

This equation has the form (22) but acts on the manifold O(3) (or rather its tangent bundle) by construction. It has not been derived, however, it has been pieced together heuristically. One can only assert that, *if* a certain system obeys a Kramers equation on a manifold, that equation may have this form.

To complete this heuristic construction we mention the additional information concerning $B_{rs}(q, u)$ that can be obtained from general physical laws. The thermodynamic equilibrium distribution

$$P^e(q, u) = \text{const.}\ |\text{Det}\ k_{rs}|^{1/2} \exp\left[-\frac{1}{\kappa T}\left\{ \frac{1}{2} k_{rs} u^r u^s + U \right\}\right]$$

must obey (39). Also, the stronger condition of detailed balance must hold, provided that there is no external magnetic field or overall rotation.

One consequence is that $B^{rs}(q, u)$ and $f^r_s(q, u)$ must be even functions of the velocities u.[23] This is important because one might have chosen for the fluctuation term in (39)

$$\frac{1}{2}\frac{\partial}{\partial u^r} B^{rs} \frac{\partial P}{\partial u^s}$$

The difference between both choices is a drift term, sometimes called the spurious drift. It now turns out to be of the same form as the friction term and may be absorbed into f^r_s. Yet this demonstrates that there is no good reason to take the f^r_s in (39) identical with the friction coefficients in the deterministic equations from which we started. This is of course the old dilemma of fluctuations in nonlinear systems[24] and can be resolved only on the basis of a more detailed study of the actual system,[25,23] as given for this case in Ref. 26.

The other consequences of detailed balance are rather involved for this general case. Normally, however, one assumes linear fluctuations, that is, B^{rs} independent of the u. In that case one obtains

$$f^r_s = \frac{1}{2\kappa T} B^{rj}(q)\, k_{js}(q)$$

which is the familiar fluctuation-dissipation relation.

APPENDIX

In $\mathbb{R}^d$ we define a metric $d\sigma^2 = B_{ij}\, dx^i\, dx^j$ where B_{ij} is the reciprocal of the coefficients B^{ij} in (18). In the new variables $\{y^r, z^\nu\}$ the transformed $\bar{B}^{kl}$ must be such that its cross elements $\bar{B}^{r\nu}$ are of order $|z|^2$. Hence, $\bar{B}_{r\nu}$ must also be of order $|z|^2$.

Choose a transformation $x^i = f^i(y, z)$ such that $z = 0$ on $\mathbb{M}$. In the neighborhood of $\mathbb{M}$

$$\begin{aligned} x^i &= f^i(y, 0) + z^\nu f^i_{,\nu}(y, 0) + \tfrac{1}{2} z^\nu z^\mu f^i_{,\nu\mu}(y, 0) + \cdots \\ &\equiv X^i(y) + z^\nu Y^i_\nu(y) + \tfrac{1}{2} z^\nu z^\mu Z^i_{\nu\mu}(y) + \cdots \end{aligned} \tag{40}$$

The variables y now simply act as parameters on $\mathbb{M}$. One has, omitting second order in z,

$$dx^i = (X^i_{,r} + z^\nu Y^i_{\nu,r})\, dy^r + (Y^i_\nu + z^\mu Z^i_{\nu\mu})\, dz^\nu$$

When $d\sigma^2$ is expressed in the new variables one finds for the coefficients in the cross terms

$$\bar{B}_{r\nu} = [X^i_{,r} + z^\mu Y^i_{\mu,r}]\, B_{ij}(\mathbf{X} + z^\lambda \mathbf{Y}_\lambda)[Y^j_\nu + z^\mu Z^j_{\nu\mu}]$$

In order that this vanishes in zeroth and first order of z one must have

$$X^i_{,r} B_{ij} Y^j_\nu = 0 \qquad \text{(all } r, \nu) \tag{41}$$

$$Y^i_{\mu,r} B_{ij} Y^j_\nu + X^i_{,r} B_{ij,k} Y^k_\mu Y^j_\nu + X^i_{,r} B_{ij} Z^j_{\nu\mu} = 0 \qquad \text{(all } r, \nu, \mu) \tag{42}$$

Here B_{ij} and its derivative $B_{ij,k}$ are taken on $\mathbb{M}$, i.e., for $x^i = X^i(y)$.

The first order (41) states that the vectors $\mathbf{Y}_\nu$ must be orthogonal (with respect to our metric in $\mathbb{R}^d$) to the $n-d$ tangent vectors $\mathbf{X}_{,r}$. They must be linearly independent for the transformation to be admissable. Of course it is easy to find n independent normal vectors at each point of $\mathbb{M}$.

The second condition (42) determines the $\mathbf{Z}_{\nu\mu}$ for each pair ν, μ, or rather the projections thereof on the tangent vectors $\mathbf{X}_{,r}$. Obviously such

$\mathbf{Z}_{\nu\mu}$ can be found, but there is the additional requirement that $\mathbf{Z}_{\nu\mu}=\mathbf{Z}_{\mu\nu}$. Hence we must have

$$B_{ij}(Y^i_{\mu,r}Y^j_\nu - Y^i_{\nu,r}Y^j_\mu)+X^i_{,r}B_{ij,k}(Y^k_\mu Y^j_\nu - Y^k_\nu Y^j_\mu)=0 \tag{43}$$

If one can find vectors $\mathbf{Y}_\nu$ that obey both (41) and (43), the $\mathbf{Z}_{\nu\mu}$ can be found from (42) and the resulting transformation (40) obeys all requirements. If no such $\mathbf{Y}_\nu$ can be found, there is no physical constraint (of the type envisaged) that leads to a diffusion equation on $\mathbb{M}$.

From now on we take isotropic, homogeneous diffusion: $B^{ij}=\delta^{ij}$. That turns out to be sufficient for constructing a counterexample. Equations (41) and (43) reduce to

$$\mathbf{X}_r\cdot\mathbf{Y}_\nu=0 \tag{44}$$

$$\mathbf{Y}_{\mu,r}\cdot\mathbf{Y}_\nu-\mathbf{Y}_{\nu,r}\cdot\mathbf{Y}_\mu=0 \tag{45}$$

Select in every point of $\mathbb{M}$ a set of n unit vectors $\mathbf{N}_\rho$ normal to $\mathbb{M}$ and to each other

$$\mathbf{N}_\rho\cdot\mathbf{X}_r=0 \qquad \mathbf{N}_\rho\cdot\mathbf{N}_\sigma=\delta_{\rho\sigma}$$

At each point y the unknown $\mathbf{Y}_\nu$ are linear combinations of them

$$\mathbf{Y}_\nu(y)=c^\rho_\nu(y)\,\mathbf{N}_\rho(y)$$

The variation of $\mathbf{N}_\rho$ with y is given by a connecting equation

$$\mathbf{N}_{\rho,r}=\omega^\sigma_{\rho r}\mathbf{N}_\sigma+\xi^u_{\rho r}\mathbf{X}_u \tag{46}$$

where $\omega^\sigma_{\rho r}=-\omega^\rho_{\sigma r}$. Condition (45) becomes

$$c^\rho_{\mu,r}c^\rho_\nu-c^\rho_{\nu,r}c^\rho_\mu+c^\rho_\mu\omega^\sigma_{\rho r}c^\sigma_\nu-c^\rho_\nu\omega^\sigma_{\rho r}c^\sigma_\mu=0$$

In terms of the matrices $C_{\nu\rho}=c^\rho_\nu$ and $(\Omega_r)_{\rho\sigma}=\omega^\sigma_{\rho r}$

$$C_{,r}C^+-CC^+_{,r}+2C\Omega_rC^+=0 \tag{47}$$

where C^+ is the transposed.

This equation is quadratic in C, but can be reduced to a linear one. First note that the following equation

$$D^+D_{,r}-D^+_{,r}D-2D^+\Omega_rD=0$$

is obeyed by both $D=C^+$ and $D=C^{-1}$. Hence if $C^+=C^{-1}$ for one value of y^r, it will be true for all values of y^r. This is achieved by taking in one point of $\mathbb{M}$ the $\mathbf{Y}_\nu$ identical with the $\mathbf{N}_\rho$. (This is no restriction because (45) is invariant for the transformation $\mathbf{Y}_\nu = a_\nu^\mu \mathbf{Y}_\mu^*$ with constant a_ν^μ.) Substituting $C^+ = C^{-1}$ in (47), one obtains the linear differential matrix equation

$$C_{,r} = -C\Omega_r \tag{48}$$

One may also note that the orthogonality of C ensures that the $\mathbf{Y}_\nu$ are orthonormal, so that (45) reduces to

$$\mathbf{Y}_{\mu,r} \cdot \mathbf{Y}_\nu = 0 \qquad \text{or} \qquad \mathbf{Y}_{\mu,r} \cdot \mathbf{N}_\rho = 0 \tag{49}$$

This leads again to (48).

If $d - n = 1$ so that r takes on only a single value, this equation can be integrated. Hence *for a curve in* $\mathbb{R}^d$ *it is always possible to find physical constraints that lead to a (one-variable) diffusion equation along that curve.* This is a local statement and applies only to simply connected curves. I do not say anything about global properties.

If $d - n > 1$, however, there is the integrability condition

$$\Omega_{r,s} - \Omega_{s,r} - \Omega_s \Omega_r + \Omega_r \Omega_s = 0 \tag{50}$$

On the other hand, we know from (46)

$$\mathbf{N}_{\rho,rs} = \omega^\sigma_{\rho r,s} \mathbf{N}_\sigma + \omega^\sigma_{\rho r}(\omega^\tau_{\sigma s} \mathbf{N}_\tau + \xi^u_{\sigma s} \mathbf{X}_u) + \xi^u_{\rho r,s} \mathbf{X}_u + \xi^u_{\rho r} \mathbf{X}_{u,s} \tag{51}$$

Multiply with $\mathbf{N}_\tau$ and define the (nonsquare) matrices Ξ_r and L_r by

$$(\Xi_r)_{\rho u} = \xi^u_{\rho r}, \qquad (L_r)_{u\tau} = \mathbf{X}_{,ru} \cdot \mathbf{N}_\tau$$

Then the fact that (51) is symmetric in r, s gives

$$0 = \Omega_{r,s} - \Omega_{s,r} + \Omega_r \Omega_s - \Omega_s \Omega_r + \Xi_r L_s - \Xi_s L_r$$

Consequently the integrability condition is tantamount to

$$\Xi_r L_s = \Xi_s L_r \tag{52}$$

It is easy to see that $L_r = -\gamma \Xi_r^+$ where $\gamma_{rs} = \mathbf{X}_r \cdot \mathbf{X}_s$ is the metric tensor of $\mathbb{M}$. Hence (52) may be written

$$L_r^+ \gamma^{-1} L_s = L_s^+ \gamma^{-1} L_r \tag{53}$$

Although the matrices L_r depend on our choice for the $\mathbf{N}_r$, the criterion itself does not.

We now give an example of a manifold for which (48) cannot be satisfied. Since we know that for $d-n=1$ and for $n=1$ it can always be satisfied, we take $d=4$, $n=2$. Consider the two-dimensional $\mathbb{M}$ defined by

$$\mathbf{X}(\alpha, \beta) = (\alpha \cos \beta, \alpha \sin \beta, \beta, \alpha) \tag{54}$$

where α, β stand for y^1, y^2. Then

$$\mathbf{X}_{,\alpha} = (\cos \beta, \sin \beta, 0, 1)$$
$$\mathbf{X}_{,\beta} = (-\alpha \sin \beta, \alpha \cos \beta, 1, 0)$$

and we choose

$$\mathbf{N}_1 = (1+\alpha^2)^{-1/2} (\sin \beta, -\cos \beta, \alpha, 0)$$
$$\mathbf{N}_2 = 2^{-1/2} (\cos \beta, \sin \beta, 0, -1)$$

Because of the orthogonality of C we may write

$$\mathbf{Y}_1 = \mathbf{N}_1 \cos \theta + \mathbf{N}_2 \sin \theta$$
$$\mathbf{Y}_2 = -\mathbf{N}_1 \sin \theta + \mathbf{N}_2 \cos \theta$$

and have to determine $\theta(\alpha, \beta)$ so as to satisfy (51). By direct substitution one obtains

$$\mathbf{Y}_{1,\alpha} \cdot \mathbf{Y}_2 = \frac{\partial \theta}{\partial \alpha}, \qquad \mathbf{Y}_{1,\beta} \cdot \mathbf{Y}_2 = \frac{\partial \theta}{\partial \beta} - \frac{1}{2\sqrt{1+\alpha^2}}$$

Clearly there exists no $\theta(\alpha, \beta)$ for which both these quantities vanish. One may also verify explicitly that (53) is not obeyed.

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