DIFFUSION EQUATION AND NON-HOLONOMY

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1. INTRODUCTION

In a previous paper (1) we have argued that the classical equations of motion for a particle subject to a non-holonomic constraint cannot be equivalent to equations derived by the vanishing of the first variation of an action functional. This result immediately raises a few questions that we will try to answer and clarify in this paper.

Hertz (2) was one of the first to question the variational principle of classical mechanics based on the non-holonomy of constraints. The original enunciation of Hamilton's principle refers specifically to holonomic systems. When one considers non-holonomic constraints the variational principle can be generalized by treating the constraints as subsidiary conditions to the first variation of the action integral. The issue usually raised around this point is whether the varied paths are among geometrically possible paths or not. A recent exposition on this old problem is given by P. Sussekind Rocha (3) in his essay on D'Alembert's principle. A better known discussion is that given by Pars (4) in answer to a similar question posed by Capon (5).

The lack of a Hamiltonian formalism for non-holonomic systems makes the quantization of such systems a very difficult task and inapplicable to standard procedures. Therefore, we have turned our attention to the analog problem of deriving the diffusion equation for such systems. Even here the problem escapes standard procedures for deriving the diffusion equation as in general Liouville's measure is not invariant.

In this paper we discuss the diffusion equation for particles in a Riemannian space subject to a single constraint. We further discuss the implications of the holonomy and non-holonomy of this single constraint.

In section two we discuss holonomy in the ligth of gauge theory and in section three we derive in a detailed way the diffusion equation for such systems. Section four does the same for the case of non-integrability of the constraint and section five studies the limit of the two equations derived when the non-integrable constraint converges to an integrable one. Section six exhibits an example obtained by simulation and in section seven we draw the conclusions of this paper.

2. HAMILTONIAN FORMALISM FOR PARTICLES SUBJECT TO HOLONOMIC CONSTRAINTS

The purpose of this section is to derive the Hamiltonian for a particle constrained to move on the surface.

$$\phi(\vec{p}) = 0, \quad \frac{\partial\phi}{\partial q^i}\frac{\partial\phi}{\partial q^i} \neq 0 \tag{2.1}$$

imbedded in a Euclidean n-dimensional space.

This is accomplished by Dirac's formalism for singular Lagrangeans.

The Lagrangean for the system may be written as

$$L = \frac{1}{2}\dot{q}^i \dot{q}^i + \alpha\phi \quad , \tag{2.2}$$

where α is a Lagrangean multiplier and must be considered a new dynamical variable, adding to the configuration a new dimension.

Since $\dot{\alpha}$ is absent from the Lagrangean, the momentum β, canonically conjugate to α, must vanish identically, i.e.,

$$\beta \equiv \frac{\partial L}{\partial\dot{\alpha}} = 0 \tag{2.3}$$

which defines a primary constraint .

We may now construct Dirac Hamiltonian, writing

$$H_D = \frac{1}{2} p_i p_i - \alpha\phi - \mu\beta \tag{2.4}$$

where μ is an undetermined function of p,q and α.
Consistency with the constraint imposes that the arbitrary function μ in H must be such that all time derivatives of β vanish. This requirement generates a new set of constraints and therefore we have:

$$X^1 \equiv \beta = 0 \tag{2.5}$$

$$X^2 \equiv \dot{\beta} = \{\beta, H_D\} = \phi = 0 \tag{2.6}$$

$$X^3 \equiv \ddot{\beta} = \frac{\partial\phi}{\partial q^i} p_k = 0 \tag{2.7}$$

$$X^4 \equiv \dddot{\beta} = \alpha \frac{\partial\phi}{\partial q^i} \frac{\partial\phi}{\partial q^i} + \frac{\partial^2 \phi}{\partial q^i \partial q^k} p_i p_k = 0 \tag{2.8}$$

$$X^5 \equiv \ddddot{\beta} \equiv \frac{\partial^3 \phi}{\partial q^\ell \partial q^k \partial q^i} p_\ell p_k p_i + 4\alpha \frac{\partial\phi}{\partial q^i} \frac{\partial^2 \phi}{\partial q^i \partial q^k} p_k - \mu \frac{\partial\phi}{\partial q^i} \frac{\partial\phi}{\partial q^i} = 0 \tag{2.9}$$

where { , } is the notation for the Poisson bracket .

The last eq. fixes the only undetermined function in the generalized Hamiltonian, eq. (2.4), exhibiting the fact that all the four constraints given by eqs. (2.5) to (2.9) are second class constraints. These four constraints reduce by four the dimension of the phase space and therefore by two the configuration space. These two dimensions of the configuration space can be seen to correspond to the additional dimension due to the inclusion of α as a new dynamical variable and the dimension corresponding to the motion in the direction normal to the surface $\phi = 0$. This is easily seen if we perform the canonical transformation generated by

$$F_2 = f^i P_i , \tag{2.10}$$

where f^i are functions of the old coordinates and P_i are the new momenta.

We define f^i as follows

$$f^i = Q^i(q) \quad \text{for } i = 1, \ldots, n-1, \tag{2.11}$$

Where Q^i are the new coordinates caracterizing the points on the surface $\phi(q) = 0$. We may choose Q^i in such a way that

$$\frac{\partial \phi}{\phi q^i} \frac{\partial Q^j}{\phi q^i} = 0 \quad , \quad j = 1,\ldots,n-1 .$$

Besides we assume

$$f^n = \phi(q) . \tag{2.12}$$

The old momenta are given by

$$p_i = \frac{\partial F_2}{\partial q^i} = \frac{\partial \phi}{\partial q^i} P_n + \frac{\partial Q^j}{\partial q^i} P_j$$

which can be solved for P_n. We get

$$P_n = \frac{1}{\frac{\partial \phi}{\partial q^j} \frac{\partial \phi}{\partial q^j}} \frac{\partial \phi}{\partial q^i} p_i$$

what shows that

$$P_n \equiv X_3 = 0.$$

From these results we see that the four eqs. $X_i=0$ eliminate the two pairs of canonical variables: (α,β) and (ϕ,P_n). The Dirac Hamiltonian in the reduced space of (P_i,Q_i), $i=1,\ldots,n-1$, is given by

$$H = \frac{1}{2} \bar{g}^{ij} P_i P_j , \tag{2.13}$$

where

$$\bar{g}^{ij}(Q) = \sum_{k=1}^{n} \frac{\partial Q^i}{\partial q^k} \frac{\partial Q^j}{\partial q^k}$$

is the metric tensor of the surface $\phi = 0$

3. DIFFUSION EQUATION FOR PARTICLES CONSTRAINED TO SURFACES

In this section we derive the diffusion equation for an ensemble of non-interacting particles, subject to white stochastic forces, moving on a surface.

We start from the Hamiltonian, obtained previously

$$H = \frac{1}{2} \bar{g}^{ij} P_i P_j$$

where $\bar{g}^{ij}$ is the metric tensor.

Hamilton's equations are

$$\dot{Q}^i = \frac{\partial H}{\partial p_i} = \bar{g}^{ij} P_j \qquad (3.1)$$

$$\dot{P}_i = - \frac{\partial H}{\partial Q^i} = - \frac{1}{2} \frac{\partial \bar{g}^{jk}}{\partial Q^i} P_j P_k . \qquad (3.2)$$

Let us assume a stochastic force acting on the particles with a white correlation:

$$\langle F^i(t) F_j(t') \rangle = 2K \delta^i{}_j \delta(t-t') \qquad (3.3)$$

and consequently,

$$\langle F_i(t) F_j(t') \rangle = \langle \bar{g}^{ik} F^k(t) F_j(t') \rangle = 2K \bar{g}_{ij} \delta(t-t'). \qquad (3.4)$$

The viscosity is introduced as the tensor

$$\gamma^i{}_j = \gamma \; \delta^i{}_j$$

what gives for the covariant force the following expression

$$f_i = - \gamma \; \bar{g}_{ij} \; \frac{\partial H}{\partial P_j} \tag{3.5}$$

From these considerations we finally arrive at the eqs. of motion:

$$\dot{Q}^i = \frac{\partial H}{\partial P_i} \tag{3.6}$$

$$\dot{P}_i = - \frac{\partial H}{\partial Q^i} - \bar{g}_{ij} \; \frac{\partial H}{\partial P_j} + F_i \; .$$

To arrive at the Fokker-Planck equation for the distribution G(P,Q,t) one must calculate the correlations of the dynamical variables at two instants of time and we obtain from eq.(3.4) and (3.6):

$$\langle \Delta Q^i \rangle = \frac{\partial H}{\partial P_i} \; \Delta t$$

$$\langle \Delta P^i \rangle = \left(- \frac{\partial H}{\partial Q^i} - \gamma \, \bar{g}_{ij} \; \frac{\partial H}{\partial P_j} \right) \Delta t$$

$$<\Delta Q^i \, \Delta Q^j> \; = \; <\Delta Q^i \; \Delta P_j> \; = \; O(\Delta t^2)$$

$$<\Delta P_i \, \Delta P_j> = 2K \, \bar{g}_{ij} \Delta t$$

with these results we write down Fokker-Planck eq. as:

$$\frac{\partial G}{\partial t} = - \frac{\partial}{\partial Q^i} \left(\frac{\partial H}{\partial P_i} \; G \right) + \frac{\partial}{\partial P_i} \left[\left(\frac{\partial H}{\partial Q^i} + \bar{g}_{ij} \frac{\partial H}{\partial P_j} \right) G \right]$$

$$+ K \, \bar{g}_{ij} \frac{\partial^2 G}{\partial P_i \, \partial P_j} \qquad ,$$

which can be rewritten in the following form:

$$\frac{\partial G}{\partial t} + \{G,H\} \; = \gamma \, \bar{g}_{ij} \frac{\partial}{\partial P_i} \left(\frac{\partial H}{\partial P_j} \, G \right) + K \, \bar{g}_{ij} \frac{\partial^2 G}{\partial P_i \, \partial P_j} \tag{3.7}$$

Obviously any function of H vanishes the left-hand side of eq. (3.7). In particular the function describing the thermal equilibrium

$$G_0(P,Q) = Z^{-1} \exp(-\beta H) \tag{3.8}$$

vanishes also the right-hand side of eq. (3.7) and is therefore the equilibrium solution of the Fokker-Planck eq. if:

$$\beta K = \gamma \tag{3.9}$$

The equation above exhibits the relation between the viscosity and the strength of the stochastic forces for a given temperature ($\beta=1/kT$). The coefficient Z is the partition function and here it plays the role of a normalizing factor.

It is important to observe that the left-hand side of eq. (3.8) describes the purely mechanical motion of the system. The remaining two terms on the right-hand side are of stochastic origin and are responsible for carrying the system to its equilibrium distribution.

Let us define the density at equilibrium as

$$\rho_0(Q) = \int \prod_{i=1}^{n-1} dP_i \; G_0(P,Q) = Z^{-1} \left(\frac{2\pi}{\beta}\right)^{(n-1)/2} \bar{g}^{1/2} = c\, \bar{g}^{1/2} . \quad (3.10)$$

The constant c is actually irrelevant to our purpose since it is related to the total number of particles put into the system, and the equations are homogeneous of the first degree. We have also set $\bar{g}=\det(\bar{g}_{ij})$.

To obtain the diffusion equation, we shall follow the same steps as in ref. (7).

We introduce an operator defined as

$$AG(P,Q,t) = \frac{G_0}{c\ \bar{g}^{1/2}} \int \prod_i dp_i G(P,Q,t) \tag{3.11}$$

where G(P,Q,t) is any function of Q,P and t. It is easy to verify that A is idempotent ($A^2=A$) and its action is to extract from any distribution function G(P,Q,t) its component that corresponds to a uniform temperature everywhere but with the same spatial distribution as given by G(P,Q,t), i.e.

$$AG = G_0(P,Q)\rho(Q,t) \tag{3.12}$$

We may rewrite the Fokker-Planck equation as

$$\frac{\partial G}{\partial t} = (\Gamma_0 + \Gamma_1)\ G \tag{3.13}$$

where

$$\Gamma_0\ G = K \frac{\partial}{\partial P_i} \left[\bar{g}_{ij} \left(\beta G \frac{\partial H}{\partial P_j} + \frac{\partial G}{\partial P_j} \right) \right] \tag{3.14}$$

and

$$\Gamma_1\ G = \{H,G\} = \frac{\partial H}{\partial Q^i} \frac{\partial G}{\partial P_i} - \frac{\partial H}{\partial P_i} \frac{\partial G}{\partial Q^i} \tag{3.15}$$

Our purpose now is to derive from eq. (3.13) a closed equation for $\rho(Q,t)$

We have:

$$G_0 \frac{\partial \rho}{\partial t} = A(\Gamma_0 + \Gamma_1)\,(G_1 + G_2) \qquad (3.16)$$

with

$$G_1 = AG \quad , \quad G_2 = BG$$

and

$$B = I - A$$

where I is the identity operator.

Let us observe that

$$\Gamma_0\, G_0 = \Gamma_1\, G_0 = 0 \qquad (3.17)$$

as already discussed.

We further have

$$\Gamma_0\, A = A\, \Gamma_0 = 0\ .$$

To see this, we take an arbitrary distribution g and we set

$$AG = G_0\, \rho\ ,$$

and therefore

$$\Gamma_0 \, AG = \Gamma_0(G_0 \, \rho) = G_0 \, \Gamma_0 \, \rho = 0$$

as Γ_0 is a differential operator only on the momentum variables.

We also have

$$A \, \Gamma_0 \, G = \frac{K \, G_0}{c \, \sqrt{\bar{g}}} \int \prod_{\ell} dP_\ell \, \frac{\partial}{\partial P_i} \left[\bar{g}_{ij} \left(\beta G \, \frac{\partial H}{\partial P_j} + \frac{\partial G}{\partial P_j} \right) \right] = 0$$

assuming that

$$P_i G \to 0 \quad \text{and} \quad \frac{\partial G}{\partial P_j} \to 0 \quad \text{as} \quad P_i \to \pm\infty$$

By similar arguments we can also prove that

$$A \quad \Gamma_1 \, A = 0 \tag{3.18}$$

Making use of eqs. (3.17) and (3.18) in eq. (3.16) we obtain

$$G_0 \, \frac{\partial \rho}{\partial t} = A \, \Gamma_1 \, G_2 \quad . \tag{3.19}$$

To proceed we must obtain the equation for G_2. Applying B to both sides of Fokker-Planck equation we get

$$\frac{\partial G_2}{\partial t} = B \, (\Gamma_0 + \Gamma_1) \, (G_1 + G_2)$$

or, again making use of eqs. (3.17) and (3.18):

$$\frac{\partial G_2}{\partial t} = (B\,\Gamma_1 + \Gamma_0)\,G_2 + \Gamma_1\,G_1. \tag{3.20}$$

The previous equation can be formally integrated as

$$G_2 = \int_0^t \exp\left[(B\,\Gamma_1 + \Gamma_0)\quad(t-t')\right]\,\Gamma_1\,G_1\;dt' \tag{3.21}$$

where we assume that $G_2=0$ at $t=0$. The meaning of this initial condition is that we start with a system in thermal equilibrium and therefore $AG = G$ at $t=0$.

Substituting eq. (3.21) into eq. (3.19) we have

$$G_0\,\frac{\partial \rho}{\partial t} = A\,\Gamma_1 \int_0^t \exp\left[(B\,\Gamma_1 + \Gamma_0)\,(t-t')\right]\,\Gamma_1\,G_1\;dt' \tag{3.22}$$

From eqs. (3.19) and (3.20) we observe that Γ_1 is the operator responsible for thermal fluctuations of the system. We make the simplifying assumption of neglecting higher order corrections in $B\Gamma_1$ and thus

$$G_0\,\frac{\partial \rho}{\partial t} = A\,\Gamma_1 \int_0^t \exp\left[\Gamma_0(t-t')\right]\,\Gamma_1\,G_1\;dt' \;.$$

It can be proved that

$$\Gamma_0 \; \Gamma_1 \; G_1 = -\gamma \quad \Gamma_1 \; G_1$$

and therefore we have

$$G_0 \frac{\partial \rho}{\partial t} = A \; \Gamma_1 \int_0^t \exp \left[-\gamma(t-t') \right] \Gamma_1 \; G_1 \; dt' .$$

We make a further simplification, by assuming $\Gamma_1 \; G_1$ to vary slowly in time intervals of the order of γ^{-1} and so we get

$$G_0 \frac{\partial \rho}{\partial t} = \frac{1}{\gamma} A \; \Gamma_1^2 \quad G_1 \; . \tag{3.23}$$

Making use of the following relations:

$$\int \prod_{\ell} dP_{\ell} \; G_0 \; P_i \; P_j = \frac{c \sqrt{\bar{g}}}{\beta} \bar{g}_{ij}$$

$$\frac{\partial \bar{g}^{ij}}{\partial Q^k} = - \bar{g}^{im} \left\{ \begin{matrix} j \\ mk \end{matrix} \right\} \quad -\bar{g}^{jm} \left\{ \begin{matrix} i \\ mk \end{matrix} \right\}$$

and

$$\left\{ \begin{matrix} i \\ ij \end{matrix} \right\} = \frac{1}{\sqrt{\bar{g}}} \quad \frac{\partial \sqrt{\bar{g}}}{\partial Q^j}$$

we finally arrive at the diffusion equation:

$$\frac{\partial \rho}{\partial t} = \frac{D}{\sqrt{\bar{g}}} \frac{\partial}{\partial Q^i} \left(\bar{g}^{ij} \sqrt{\bar{g}} \frac{\partial \rho}{\partial Q^j} \right) \tag{3.24}$$

where

$$D = 1/(\gamma\beta) \tag{3.25}$$

The operator on the rigth-hand side of eq. (3.24) is the Laplacian operator in the Riemannian space and D is the diffusion coefficient.

It is important to observe that eq. (3.24) is the diffusion equation not only for particles moving in a generalized configuration space with metric given by the tensor g_{ij} but is also for particles subject to arbitrary holonomic constraints, as the elimination of the constraints always leads to a Hamiltonian unconstrained motion in a reduced configuration space with a modified metric.

4. DIFFUSION EQUATION FOR PARTICLES SUBJECT TO NON-INTEGRABLE CONSTRAINTS

Let us begin by considering the Lagrangean

$$L = \frac{1}{2} g_{ij} \dot{q}^i \dot{q}^j - \lambda a_i \dot{q}^i \tag{4.1}$$

which describes a particle in a Riemannian space, subject to the constraint

$$a_i \dot{q}^i = 0 \tag{4.2}$$

Without loss of generality we may assume that

$$a_i a^i = 1$$

Proceeding similarly to what we have done in section 2, we obtain as primary constraint the equation

$$\Pi = 0$$

where Π is the canonical momentum conjugate to λ and , as secondary constraint the following equation

$$\lambda + a^i p_i = 0 .$$

These last two equations can be used to eliminate Π and λ from the extended Hamiltonian and we obtain

$$H = \frac{1}{2} g^{ij} Q^k_j p_i p_k \tag{4.3}$$

where

$$Q^i{}_j = \delta^i{}_j - a^i a_j \tag{4.4}$$

So far we have not made use of the fact that $a_i\dot{q}^i$ is not integrable. Let us first assume that $a_i\dot{q}^i$ is integrable, i.e.

$$a_i = \tau \frac{\partial\phi}{\partial q^i}$$

where ϕ is the integral of eq. (4.2) and τ is the integrating factor. In this case we have

$$\{\phi , H\} = 0$$

and ϕ plays the role of a generator of gauge transformations and must be treated as a first class constraint for the system described by H.

The transformations generated by ϕ are

$$\delta q_i = \varepsilon\{q^i, \phi\} = 0$$

$$\delta p_i = \varepsilon\{p_i, \phi\} = - \varepsilon \frac{\partial\phi}{\partial q_i} = - \varepsilon \tau^{-1} a_i$$

and therefore ϕ changes only the component of p parallel to a. Thus we choose as gauge condition the equation

$$a^i p_i = 0$$

The equation above, together with the equation

$$\phi = 0$$

can be used to reduce the phase space of the system by a canonical transformation in which ϕ plays the role of the n-th variable similarly to what we have done in section 2.
The Hamiltonian in the reduced space have the form

$$H^* = \frac{1}{2} \bar{g}^{\alpha\beta} p_\alpha p_\beta \qquad \alpha,\beta = 1,\dots,n-1$$

where

$$(g_{ij}) = \left(\begin{array}{c|c} (\bar{g}_{\alpha\beta}) & 0 \\ \hline 0 & \left(\dfrac{\partial\phi}{\partial\phi^1}\right)^2 \end{array} \right)$$

and H^* is the same as the one given by eq. (2.13) and therefore the diffusion equation is given by the eq. (3.23) as was shown in the previous section.
If the eq. (4.2) is not integrable, no further invariance appears in the system and we have to deal with the Hamiltonian H given by eq. (4.3) defined in the whole 2n - dimensional phase space. The presence of the constraint is manifested by the fact that the metric

$$\tilde{g}^{ij} = g^{ik} Q^j_k$$

is singular. To overcome this difficulty we consider the system described by the following Hamiltonian

$$H(\varepsilon) = \tilde{g}^{ij}(\varepsilon)\, p_i\, p_j \tag{4.5}$$

with

$$\tilde{g}^{ij}(\varepsilon) = g^{ik}\, Q_k^j\, (\varepsilon) \tag{4.6}$$

and

$$Q_k^j\, (\varepsilon) = \delta_k^j - (1-\varepsilon)\, a^j a_k$$

with this procedure the metric given by eq. (4.6) is no longer singular and

$$\tilde{g} = \det\, (\tilde{g}_{ij}) = g/\varepsilon$$

With this modification the steps described in section 3 can be reproduced and we arrive at the diffusion equation

$$\frac{\partial \rho}{\partial t} = D\, \frac{1}{\sqrt{\tilde{g}}}\, \partial_i\, (\sqrt{\tilde{g}}\, g^{ij}\, Q_j{}^k(\varepsilon)\, \partial_k \rho)$$

and we observe that the limit when $\varepsilon \to 0$ exists and is :

$$\frac{\partial \rho}{\partial t} = D\, \frac{1}{\sqrt{g}}\, \partial_i\, (\sqrt{g}\, g^{ij}\, Q_j^k\, \partial_k \rho) \tag{4.7}$$

which is the equation that describes the diffusion of a particle subject to the non-integrable constraint $a_i \dot{q}^i = 0$, which is structurally different from eq.(3.23) for integrable constraints.

5. HOLONOMY AS A BIFURCATION SET FOR THE CONSTRAINED DIFFUSION EQUATION

We will now discuss the behaviour of eq. (4.7) when the cons - traint becomes integrable.
Let us first consider the space spanned by all 1-forms in a n-dimensional Riemannian manifold.

To every 1-form $\omega = a_i dq^i$, we have a constrained mechanical system and we are interested in how one system changes into another as we change the constraint continuously. One can introduce in the space of forms a topology* that guarantees the convergence of the exterior derivative and the exterior product implying therefore that the set of integrable 1-forms is closed. This is easily seen using Froebenius theorem which says that ω is integrable if and only if

$$\omega \wedge d\omega = 0$$

Thus, if ω_n is a sequence of integrable 1-forms that converges to ω then

$$\omega_n \wedge \omega_n = 0 \Longrightarrow \omega \wedge d\omega = 0$$

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* For example the topology in the space of 1-forms induced by the following distance

$$d(\omega,\omega') = \sup_{\substack{x,n \\ \{i,i_q,\dots,i_n\}}} \left\{ \left| \frac{\partial^n (a_i - a'_i)}{\partial q_{i_1} \dots \partial q_{i_n}} \right| \right\}$$

what proves that the set of integrable forms is closed.

If ω is integrable and ξ non-integrable then

$$\omega_n = \omega + \frac{1}{n} \xi$$

is non-integrable. Thus, every integrable 1-form ω can be reached by a sequence of non-integrable 1-forms what shows that the set of integrable 1-forms does not have interior what shows that it is a meagre subset of the set of 1-forms.

These results justify to take the limit in the diffusion eq.(4.7) for the non-integrable constraint and we have

$$\frac{\partial \rho}{\partial t} = D \frac{1}{\sqrt{g}} \partial_i \left(\sqrt{g} g^{ij} Q_j^{\ k} \partial_k \rho \right)$$

with the only difference that

$$a_j = \tau \frac{\partial \phi}{\partial q^j}$$

and

$$\tau^2 g^{jk} \frac{\partial \phi}{\partial q^j} \frac{\partial \phi}{\partial q^k} = 1$$

Under these assumptions one can prove that if ρ is a solution of the equation above, $\rho f(\phi)$ is also a solution .
To study the limit of the integrable case we set :

$$f(\phi) = \delta(\phi) .$$

as a necessary boundary condition.

Now we can take tha coordinate system such that $q_n = \phi$. In this case we have

$$\left(g_{ij}\right) = \left(\begin{array}{c|c} \bar{g}_{\alpha\beta} & 0 \\ \hline 0 & g_{nn} \end{array}\right)$$

with

$$g_{nn} = \frac{\partial\phi}{\partial q_i} \frac{\partial\phi}{\partial q_i}$$

and

$$\rho = \bar{\rho}(q_1 \ldots q_{n-1}) \; \delta(\phi) .$$

Substituting this into equation (4.7) we have:

$$\frac{\partial\bar{\rho}}{\partial t} = D \frac{1}{\sqrt{\bar{g}} \; \sqrt{g_{nn}}} \partial_\alpha \left(\sqrt{g_{nn}} \; \sqrt{\bar{g}} \; g^{\alpha\beta} \; \partial_\beta \bar{\rho} \right)$$

This equation, except for the special case in which g_{nn} is constant, does not coincide with the correct equation for the diffusion with holonomic constraint obtained in section 3.

We may therefore conclude that the holonomic mechanical systems are bifurcation points for the diffusion equation for general constrained systems.

6. AN EXAMPLE .

To illustrate the previous result, let us consider the diffusion of particles subject to the non-integrable constraint

$$w' + \alpha w'' = 0$$

dependent on a parameter α and in which

$$w' \equiv \frac{x_1 dx_1 + x_2 dx_2}{\beta^2} + \frac{x_3 dx_3}{\gamma^2} = 0 \qquad (6.1)$$

The leaves of the foliation given by eq. (6.1) are ellipsoids of revolution around the x_3 - axis with γ/β being the ratio of the ellipsoids axes. We consider only the equilibrium dis - tribution and we can easily see that the eq.(4.7) has in this case the solution

$$\rho = \text{const.}$$

so long as the constraint remains non-integrable . In the limit $a \to 0$, the density stays constant on each leaf and we set

$$\rho = \text{const}\ \delta(\phi)$$

on the leaf $\phi=0$ of w'.

The predicted surface density on $\phi = 0$ is therefore

$$\begin{aligned} \rho d\sigma &= d\sigma \int \text{const}\ |\nabla\phi|\,\delta(\phi)\, d\phi \\ &= \text{const}\ |\nabla\phi|\, d\sigma \qquad \text{for } \phi=0 \qquad (6.2) \end{aligned}$$

On the other hand, the surface density predicted by eq.(3.24) is

$$\rho d\sigma = \text{const } d\sigma. \qquad (6.3)$$

and we observe a clear disagreement between the two predictions when $|\nabla\phi|$ is not constant. This is so because as we observed in the previous section the diffusion equation for non-integrable constraint does not converge to the diffusion equation for the integrable case.

To illustrate further this fact we simulated the statistical equilibrium of particles on the ellipsoid given by

$$9\,(x_1^2 + x_2^2) + x_3^2 = 9 \qquad (6.4)$$

The simulation was made by considering one particle moving on the surface of the ellipsoid suffering collisions with other particles of equal mass and given temperature (β=1) . The collisions occured at every unit of time interval and the particle was observed after each collision, fourty thousand times. We considered these observations of the same particle at constant intervals of time as representatives of the canonical ensembles and the projected density of particles on the x_3-axis and the equatorial plane were observed.

In fig. (1) we exhibit our data for the particle distribution as a function of x_3 together with the two predictions given by eqs. (6.2) and (6.3). The simulation data are plotted as circle points and the predictions given by eq (6.3) and eq (6.2) are represented respectively by the continuous and the dashed curves. We clearly see that the data agree with the prediction of eq. (6.3) what shows that the diffusion eq. for a non-integrable constraint gives the wrong limit when the constraint converges to an integrable one.

We can understand these results in a simple way by considering Fig. 2. The integrable case predicts a constant surface density. By considering the volume between two ellipsoids of the same foliation we can argue that to have a constant volumetric density on the equatorial plane implies a different volumetric density at the poles. Therefore, the constant volumetric density everywhere predicted by the diffusion equation for non-integrable constraint cannot be reproduced when the constraint is integrable. In physical systems in which the non-integrable constraint changes to an integrable one, we would suddenly observe a change in the spatial distribution of particles when the constraint became integrable. We must observe on the other side that the Hamiltonian description for non-integrable constraint does not give the correct dynamical equations and the discontinuous behaviour may not correspond to the actual physical situation.

7. CONCLUSION

We have derived the diffusion equation for holomomic constraints, eq. (3.24), and non-holonomic constraints, eq. (4.7), under the assumption that the dynamics for the non-holonomic case is given by Hamilton's principle.

Though Hamilton's principle does not give the same dynamics, it is a natural extension of the dynamics of holonomy into the realm of non-holonomy. We say natural in the sense that the non-holonomic equations of motion go continously into the holonomic ones. This does not guarantee the continuation of the diffusion equations for the two classes of constraints. In fact we have shown that the holonomic set of constraints is a bifurcation set for the diffusion equation. This immediatly raises the question as to the nature of the diffusion equation for the true non-holonomic dynamics. In a previous paper (7) we showed , for a restricted class of non-holonomic systems, those for which Liouville's measure is invariant, that the true dynamics gives the same diffusion equation as the one obtained by Hamiltonian dynamics. Unfortunately this class is too restricted to permit a generalization. Therefore , the derivation of the diffusion equation for the true dynamics remains an open problem.

FIGURE CAPTIONS

Fig. 1 - The particle distribution for the constraint given by eq. (6.4). The horizontal scale is x_3/γ . The simulation data are plotted as black circles. The continuous curve is the theoretical prediction given by eq. (6.3), and the dashed curve is the prediction given by equation (6.2)

Fig. 2 - The section of two ellipsoids of the same folliation given by eq. (6.1). The shaded areas are the cross-sections of two volumes with the same basis on the ellipsoids. We can observe that the equatorial volume is smaller than the polar one.

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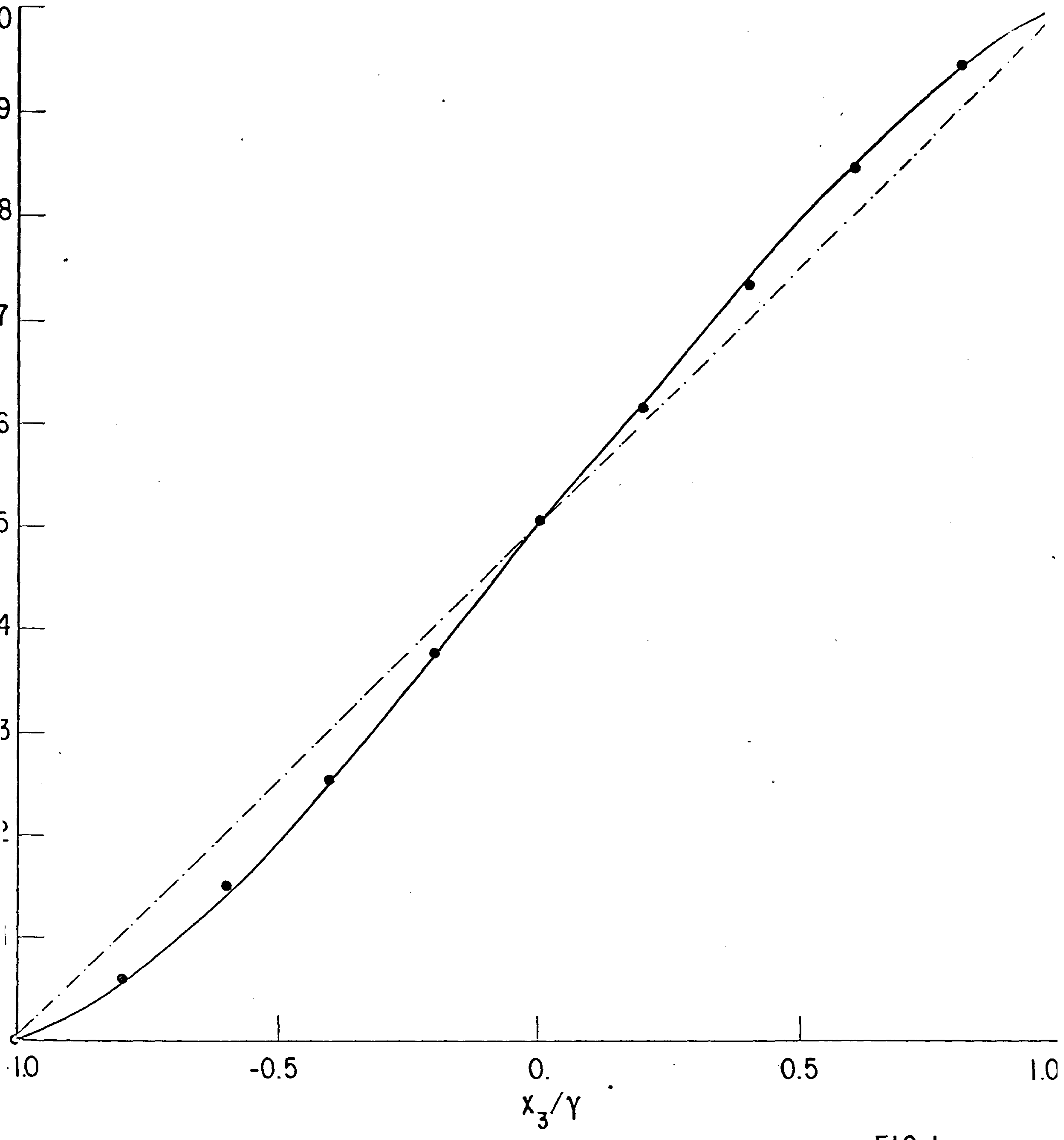

FIG. 1

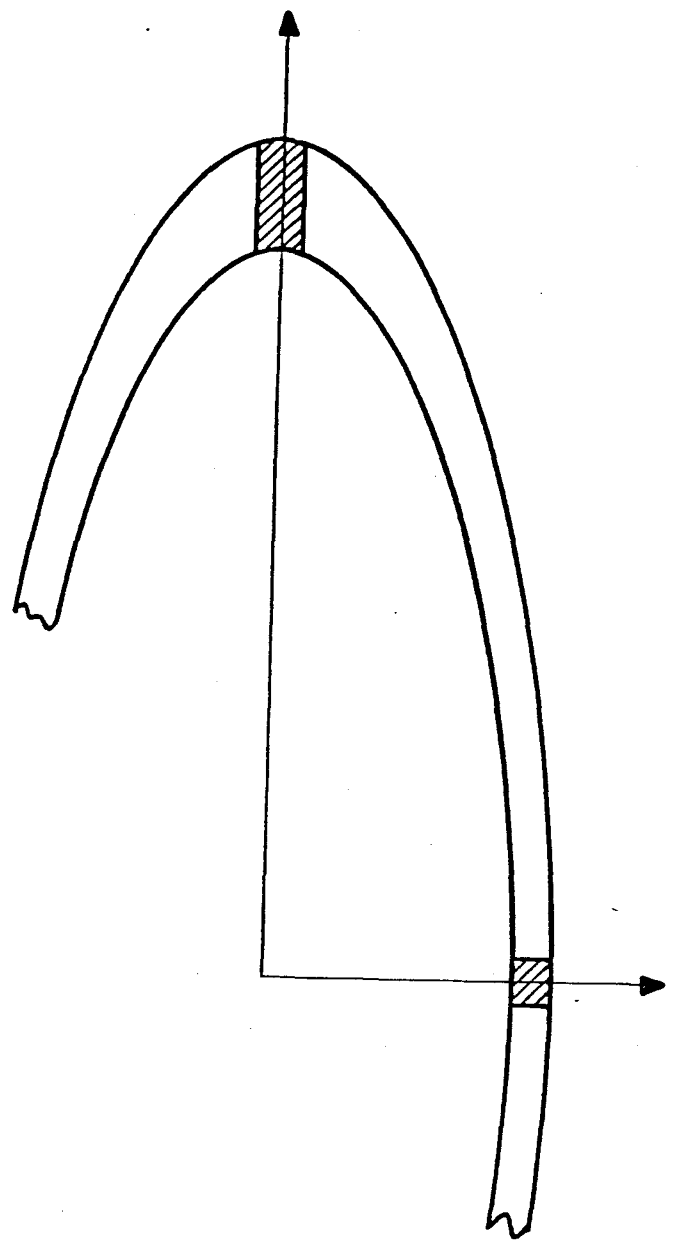

FIG. 2