Acta Universitatis Carolinae. Mathematica et Physica

K. S. Sarkaria

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Acta Universitatis Carolinae. Mathematica et Physica, Vol. 43 (2002), No. 1, 57--63

Persistent URL: `http://dml.cz/dmlcz/142717`

Stationary States

K. S. SARKARIA

Chandigarh

Received 26. June 2001

A bound frictionless microsystem has as model a closed Riemannian manifold M, i.e. its mechanics is translated into the topology and geometry of M. A stationary state of the microsystem is thought of as a coherent flow of micromatter on M, and the energy levels of the microsystem are interpreted in terms of the topological nature of this flow. A crucial hypothesis made is that a cohomology class defined by this flow must be combinatorially realizable via some triangulation K of M. (One can think of this simplicial complex K as modelling the fine-grained discrete nature of micromatter, with M being a continuous visualisation obtained by using the real numbers.) We show that this geometric model is related in a simple way with the Schrodinger equation of the microsystem.

Our perceptions seem to depend on our concepts and conversely; or, as a Deist would have it, the same tendencies which shaped the external world are responsible for our abstract concepts.

Be it as it may, a geometer perhaps perceives a natural phenomenon as a sequence $M_1 \supseteq M_2 \supseteq \ldots \supseteq M_n \supseteq \ldots$ of manifolds, each of dimension smaller than the previous, each stage corresponding to a more precise comprehension. If one finally gets down to a zero dimensional manifold, one has acheived exact determination of the phenomenon.

To take an example, in analytical mechanics we pick up this process at a stage when we have decided that all the *possible configurations* of the system are represented by points of a smooth finite dimensional manifold M. We shall use the word "system" to connote the phenomenon together with all the boundary conditions, e.g. the measuring devices. Furthermore we will suppose that this physical system is conservative. This amounts to assuming that M, and the geometrical structure which we will put on M to go to more precise stages in our

Department of Mathematics, Panjab University, Chandigarh 160014, India

mental process, do not depend on time. We remark that $m = \dim(M)$ is generally equal to the degrees of freedom of the system; but, in some special cases it might be bigger. We will think of time as a one dimensional continuum $\mathbb{R}$ and, to start with, we think of any smooth function $f\colon \mathbb{R} \to M$ as a *possible motion* of the system. In case when m is bigger than the number of degress of freedom, one can select a sub tangent bundle $D \subset T_M$, and rule out of the realm of possible motions those functions f which are not always tangent to D. The fibre dimension of D equals the degrees of freedom. But D is not integrable; in fact the totality of its integral curves is M – that is why we could not start off with a manifold of smaller dimension.

One can say that knowledge of the exact configuration of the system amounts to knowing a Dirac delta function on M, the "function" being nonzero at the point of M in question.

In continuous mechanics, though the degrees of freedom is infinite, a similar finite dimensional configuration space M can be used if one considers a possible configuration as a smooth measure on M (instead of a Dirac distribution).

So the kinematics of the system is abstracted as a smooth finite dimensional manifold. In this geometrical process of visualisation the dynamics of the system becomes a geometrical structure on M. Just as kinematics and topology are two sides of the same coin so are dynamics and geometry. It is such a tautology that is put forth by the "law" of inertia: "a body moves in a straight line with uniform

From a point
within it one sees
only local features of M.

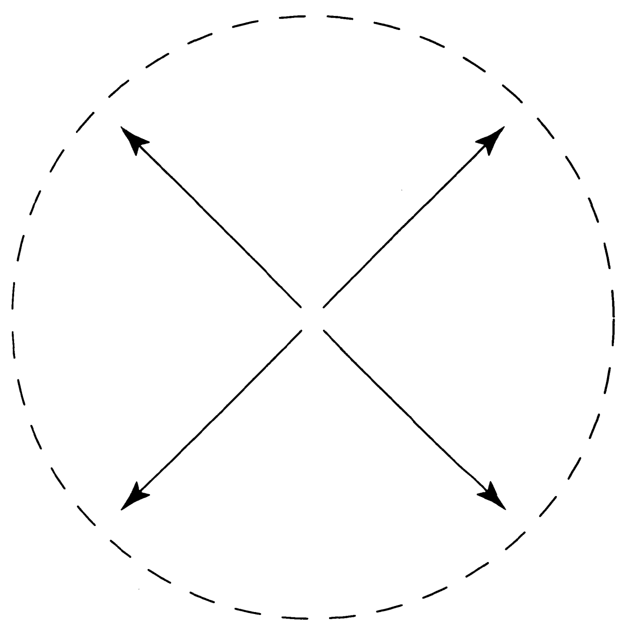

Fig. 1

motion". In fact this sentence makes sense only if one is visualising motion in a space equipped with some sort of connection. We will assume as usual that the dynamics of the system is expressed by a Riemannian connection on M. When one has reached this stage of perception, the set of all possible motions is reduced only to those functions $f: \mathbb{R} \to M$ which are geodesics, i.e. "straight lines" in the given connection. In particular at this stage one is enabled to explain how the system, starting with given positions and velocities, moves in the space M.

But in many cases, e.g. in microphenomena, one cannot accurately measure the positions and velocities at time $t = 0$, and the knowledge of this Riemannian manifold is not a "deterministic" model. In such cases the "measurable quantities" are rather obtained by performing suitable integrations over all of M, i.e. we are concerned only with properties in the large. The following pictures might help such a visualisation.

From well outside it
we see only some global
features of M.

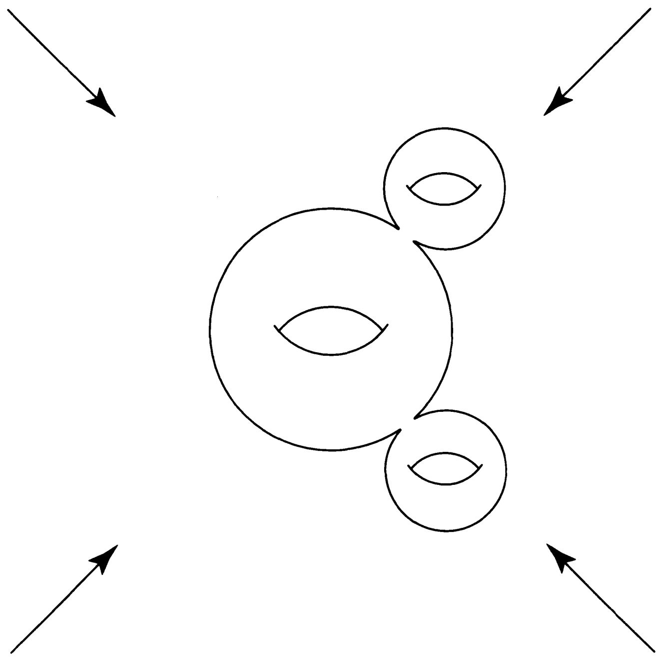

Fig. 2

Here M is closed so as to correspond to the fact that physically the microphenomenon is "bound". So a (bound) *microsystem*, as far as its mechanics (kinematics + dynamics) is concerned, is a closed Riemannian manifold of dimension m (with, if needed, some potential function).

We will assume that this microsystem is "continuous". So there is a sort of *microfluid* distributed on M according to some rule: if one knows this density function one knows the "configuration" of the microsystem.

In this picture a *stationary microflow* will be represented by a smooth tangent vector field X on M, with X not depending on time. The integral curves of X are the paths of motion of the microfluid. Since X is independent of time, on any given region of M the flow evolves in the same fashion for all time. The *law of inertia* now gives us the equation

$$\nabla_X X = 0. \tag{1}$$

Next it is natural to assume that in such a stationary state the micromatter is spread uniformly on M. We shall assume that M is orientable and that the mass is spread uniformly with respect to the volume form μg of our Riemannian metric g. Now the *equation of continuity* for this fluid motion reads

$$L_X(\mu g) = 0, \tag{2}$$

i.e.

$$\operatorname{div} X = 0. \tag{2a}$$

Let us look now at the real function $M \to \mathbb{R}$ defined by $p \mapsto \langle X(p), X(p) \rangle$. This function is constant on each integral curve of X. We will assume that our stationary microflow is *ergodic*. This implies in particular that this function must be a constant. Hence we would have an equation

$$\langle X, X \rangle = e. \tag{3}$$

The constant e will be called the *energy level* of the stationary flow. We note that we could have introduced the hypothesis that one of the orbits our flow is dense (instead of ergodicity) to get (3); but on physical grounds ergodicity seems to be a natural hypothesis (we note, by virtue of (2) and a theorem of Poincaré, that our flow X was already recurrent). By introducing ergodicity we have replaced the equation

$$\frac{1}{|M|} \int_M \langle X, X \rangle \cdot \mu g = e \tag{3a}$$

by the simpler equation (3).

Corresponding to the vector field X we have the 1-form ω_X defined by $\omega_X(Y) = \langle X, Y \rangle$. We shall say that our flow X is *coherent* if

$$\mathrm{d}(\omega_X) = 0. \tag{4}$$

Now we will examine the consequences of this condition.

Proposition 1. *The conditions (4) and (3) imply (1).*

Proof. We recall (see e.g. [1], p. 149) that for a torsionless connection $d = A \cdot \nabla$ where A is alternation and ∇ denotes covariant differential. So equation (4) says that for all vector fields Y and Z,

$$\begin{aligned} 0 &= 2(\mathrm{d}\omega_X)(Y, Z) = (\nabla_Z \omega_X)(Y) - (\nabla_Y \omega_X)(Z) = \\ &= Z(\omega_X(Y)) - \omega_X(\nabla_Z Y) - Y(\omega_X(Z)) + \omega_X(\nabla_Y Z). \end{aligned} \tag{4a}$$

Now let us put $Y = X$ in this equation. Using (3) it follows that $\omega_X(X)$ is constant, so the first term is zero. Again the second term is equal to $\langle X, \nabla_Z X\rangle = \frac{1}{2}Z(\langle X, X\rangle)$ and so this too is zero. So we get $0 = -X\langle X, Z\rangle + \langle X, \nabla_X Z\rangle = -\langle \nabla_X X, Z\rangle - \langle X, \nabla_X Z\rangle + \langle X, \nabla_X Z\rangle = -\langle \nabla_X X, Z\rangle$. Since this equation holds for all Z we see that $\nabla_X X = 0$. *q.e.d.*

We will denote by $X^\perp$ the codimension one sub bundle of T_M formed by tangent vectors perpendicular to X.

Proposition 2. *The equation (4) implies that $X^\perp$ is integrable.*

Proof. We use equation (4a) and put Y and Z as sections of $X^\perp$. Then the first and third terms vanish. Again, since $\nabla_Z Y - \nabla_Y Z = [Z, Y]$ we get the result

$$\langle X, [Z, Y]\rangle = 0 \tag{4b}$$

which shows that $[Z, Y]$ is also a section of $X^\perp$. Since $X^\perp$ is thus involutive the result follows. *q.e.d.*

Proposition 3. *If (1) and (3) hold and $X^\perp$ is integrable then the flow X is coherent.*

Proof. We have to show that (4a) is true for all vector fields Y and Z. Now if Y and Z are sections of $X^\perp$ so is $[Y, Z]$ and equation (4a) is just (4b) which is true. So we only need to verify (4a) when Y is a section of $X^\perp$ and Z is of the form fX where f is a smooth function on M. The right side of (4a) reads

$$fX\langle X, Y\rangle - \langle X, f\nabla_X Y\rangle - Y\langle X, fX\rangle + \langle X, \nabla_Y fX\rangle.$$

Clearly the first term is zero. As for the second it equals $-f\langle X, \nabla_X Y\rangle = f\langle \nabla_X X, Y\rangle$ because $\langle X, Y\rangle = 0$. So by (1) this equals zero. The third term equals $-(Yf)\langle X, X\rangle$ because by (3), $\langle X, X\rangle$ is a constant. The last term equals $\langle X, (Yf)X\rangle + \langle X, f\nabla_Y X\rangle$. But $\langle X, \nabla_Y X\rangle = \frac{1}{2}Y\langle X, X\rangle = 0$. So this term cancels with the third. *q.e.d.*

From now on we will assume that the flow X is coherent, and to thek codimension one foliation which is perpendicular to X we will give the name *stationary wave.*

Since $\iota_X(\omega_X) = \langle X, X\rangle$ is a constant we note that $L_X\omega_X = \iota_X\, d\omega_X + d\iota_X\omega_X = 0$. This implies that the one parameter group of diffeomorphisms of X carries leaves into leaves.

We can write the equation (2a) also as

$$\delta(\omega_X) = 0 \tag{2b}$$

where δ denotes the codifferential. So equations (2) and (4) can be combined into the statement that ω_X – or X – is *harmonic*; this word covers both the equation of continuity and the coherence of our flow.

Now, by a theorem of Hodge, the real vector space of all harmonic 1-forms is isomorphic to $H^1(M; \mathbb{R})$, the 1-dimensional cohomology of M with real coefficients. Not all of these classes can be defined by using only whole numbers of simplices of a simplicial triangulation K of the manifold M. These integral or combinatorially realizable classes form a lattice in this vector space $H^1(M; \mathbb{R})$. We shall say that X is *realizable* if ω_X represents such a cohomology class.

Definition. Let M be an orientable Riemannian manifold. A vector field X on M which is harmonic, "ergodic" and realizable is called a *stationary state* of M. Or, of the microsystem whose mechanics is given by M. We note that the energy levels are thus countable in number; hence we get the discrete levels which are so characteristic of microsystems. In this definition the word "ergodic" only means that $\langle X, X\rangle$ is a constant function.

Let us suppose now that U is an open contractible subset of M. Since $\mathrm{d}\omega_X = 0$ we can employ Poincaré's lemma to find on U a smooth function S such that $\mathrm{d}S = \omega_X$. We recall that for a function f its gradient $\mathrm{grad}(f)$ is a tangent vector field defined by $\langle \mathrm{grad}(f), Y\rangle = \mathrm{d}f(Y)$. Hence $\mathrm{grad}(S) = X$. Hence our equations (3) and (2b) can be written as

$$\langle \mathrm{grad}(S), \mathrm{grad}(S)\rangle = e, \tag{3b}$$

$$\Delta S = 0. \tag{2c}$$

Here, as usual, $\Delta = \delta d$ is the Laplace operator; if our metric were Euclidean then

$$\Delta = -\sum \frac{\partial^2}{\partial x_i^2}$$

in local coordinates $(x_1, \ldots, x_i, \ldots, x_m)$.

Proposition 4. *A function S satisfies the differential equations (3b) and (2c) if and only if the function $\psi = \exp(2\pi i S)$ satisfies*

$$\frac{1}{4\pi^2}\Delta\psi = e\psi. \tag{5}$$

We shall say that the equation (5) is the *Schrödinger equation* (compare e.g. with [2], p. 69) of the microsystem.

Proof. We recall that $\delta\omega_Z$ is a function which, at each point, is the trace of the linear tensor map $Y \mapsto \nabla_Y Z$. We use this with $Z = \mathrm{grad}(\psi) = 2\pi i \cdot \exp(2\pi i S) \cdot \mathrm{grad}(S)$ to see that $\Delta\psi = 2\pi i\psi\,\Delta S + \mathrm{Trace}\,[Y \mapsto 4\pi^2\psi\langle \mathrm{grad}\, S, Y\rangle\, \mathrm{grad}\, S] = 2\pi i\psi\,\Delta S + 4\pi^2\psi\langle \mathrm{grad}\, S, \mathrm{grad}\, S\rangle$. Hence the real part of (5) is (3b) and the imaginary part is (2c). *q.e.d.*

We note that on a contractible open set U a function S satisfying $\mathrm{grad}(S) = X$ is unique upto an additive constant; so the function ψ is unique upto a multiplicative constant of absolute value one.

Proposition 5. *We can have a stationary state with energy level e if and only if $4\pi^2 e$ is an eigenvalue of $\Delta : C^\infty(M) \to C^\infty(M)$ and has an eigenfunction with absolute value 1.*

Proof. Take any point $q_0 \in M$ and an open cell $V_0 \ni q_0$. Choose any function S_0 on V_0 such that $dS_0 = \omega_X$ on V_0, X being the given stationary state on M. Let us now cover M by the open cells $V_0, V_1, \ldots, V_n$; and choose one point q_i in each V_i. We now choose a function S_i on V_i such that $dS_i = \omega_X$ and

$$S_i(q_i) = S(q_0) + \int_{\gamma_i} \omega_X .$$

Here γ_i is any singular 1-simplex with vertices q_0 and q_i, i.e. γ_i; $I \to M$ is continuous with $\gamma_i(0) = q_0$, $\gamma_i(1) = q_i$.

Since ω_X defines an integral cohomology class we can say that $\int_\Theta \omega_X$ is an integer whenever Θ is a singular 1-cycle. This remark shows that in $V_i \cap V_j$, $S_i - S_j \in \mathbb{Z}$. So we can define a smooth function ψ on M which equals $\exp(2\pi i S_j)$ on V_j. By Prop. 4 this is the required eigenfunction.

Conversely, if such an eigenfunction is known, on each open cell V_j we can find a smooth real function S_j such that $\exp(2\pi i S_j) = \psi$ and define X to be the tangent vector field on M which equals $\mathrm{grad}(S_j)$ on V_j. By Prop. 4, X must be harmonic and with energy level e. *q.e.d.*

An the referee has so kindly pointed out, the above ideas are close to those on pages 130 – 132 of Nelson [3], and the author hopes to elaborate on this connection in a sequel to this paper.

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