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1974 J. Phys. A: Math. Nucl. Gen. 7 1829

(http://iopscience.iop.org/0301-0015/7/15/006)

J. Phys. A: Math., Nucl. Gen., Vol. 7, No. 15, 1974. Printed in Great Britain. © 1974

Lagrangian quantum theory III. Coordinate-free formulation

F J Bloore and L Routh

Department of Applied Mathematics and Theoretical Physics, The University, Liverpool L69 3BX, UK

Received 9 April 1974

Abstract. We show that the Fréchet derivative, which we have previously used to formulate a quantum-mechanical version of Hamilton's principle of stationary action, suffers from certain defects. The algebra of quantum observables is a quotient algebra of a free algebra of coordinate and momentum observables by its ideal generated by the canonical commutation relations. A Fréchet derivative $\delta_{\epsilon X}$ is well defined on the free algebra but passes to the quotient only if its associated vector field X is a parallel vector field. We show that one may avoid the apparently consequent restriction of the class of allowable variations in the action principle to parallel vectors by defining the variations directly on the quotient algebra. It is then not usually possible to use the notation of the Fréchet derivative. We set up a simpler, coordinate-free, formulation of quantum mechanics based on the Lie algebra of symmetric contravariant tensor fields on the configuration manifold of the system and re-express the principle of stationary action using this formalism. We find the same relation between Hamiltonian and Lagrangian as before, but a much larger class of allowable variations, namely those associated with any C^∞ vector fields.

1. Introduction

In the first two papers of this series (Bloore *et al* 1973, Bloore and Routh 1973, to be referred to as I and II) we propose a calculus of variations which appeared appropriate for a non-Abelian algebra. It was based on the Fréchet derivative and was applied to discuss Hamilton's principle in quantum mechanics. We worked in an arbitrary, but particular, coordinate system. This has a number of disadvantages. One must check the explicit covariance of one's expressions under transformation of coordinates. The formulation will hold only for systems whose configuration manifolds admit a global coordinate system. Whereas classical dynamics is a local theory, describable using a patchwork of local coordinate systems, quantum dynamics is a global theory in that states cannot be constrained to have support only in a single coordinate patch, and also in that the algebraic properties of the quantum-mechanical observable which corresponds to a function on the configuration manifold depend on all the values of the function throughout its domain, and not just on the local behaviour. Thus when the configuration manifold does not possess a global coordinate system one is forced to formulate quantum mechanics in a coordinate-free way. Such a formulation is presented in § 3. It is incomplete because there are a number of unsolved problems. However, enough of the formulation exists to present and solve the problem posed in II, namely the formulation of Hamilton's principle for an arbitrary quantum-mechanical system. This is done in § 4.

In the new formulation, the physical meaning of the coordinate and velocity observables q^i and $\dot{q}^j$ is clearer and the technical problems of evaluating commutators are much simplified and shortened.

In § 2 we present a critique of the usefulness of the Fréchet derivative. The algebra of q and $\dot{q}$ is presented as the quotient of the free algebra over the complex numbers of polynomials in the q and $\dot{q}$ by its ideal generated by the commutation relations. All Fréchet derivatives are well defined derivations on the free algebra but only a few 'pass to the quotient' as derivations, ie preserve cosets under the equivalence relations defined by the commutation relations. Each path variation $q^i(t) \to q^i(t) + \epsilon(t)X^i(q(t))$ for which the Hamiltonian action is presumed stationary corresponds to a vector field X on the configuration manifold. For Hamilton's principle fully to determine the motion of the system, there must be as many independent variations as the dimension (n) of the configuration manifold. If a variation is to specify a derivation on the quotient algebra then the corresponding vector field X must be parallel. However, if the configuration manifold admits n independent parallel vector fields then it must be flat! To avoid this crushing restriction, we show in § 3 that in each coset of the free algebra there is one element in 'normal form' and we specify the variation as a coset map by defining it on this element. We thus obtain a well defined *mapping* on the quotient algebra, but not a derivation. Although this procedure may be carried out also in the coordinate-dependent formulation, it is much easier to express and to understand in the coordinate-free formulation. With these redefined variations we find that there is a Lagrangian whose action is stationary for variations corresponding to *all* vector fields, and not just the Killing fields we obtained in II.

2. Critique of the Fréchet derivative

In this section we show that for a quantum-mechanical system, if: (i) the action is stationary with respect to sufficiently many variations that the corresponding Euler–Lagrange equations determine the motion of the system; and (ii) these variations are derivations on the algebra of observables; then the configuration space is flat.

Any description of the Hamiltonian time dependence of quantum-mechanical observables (QMO) in terms of a principle of stationary action requires a calculus of variables on the algebra of these QMO. The non-commutativity of the observables with each other led us to introduce what we called in II a Fréchet derivative on the free algebra $\mathscr{B}$ of polynomials in the QMO with complex coefficients. If the QMO corresponding to the coordinates and velocities of a system with n degrees of freedom are $q^1, \ldots, q^n$, $\dot{q}^1, \ldots, \dot{q}^n$ and $f(q, \dot{q})$ and $h(q, \dot{q})$ are polynomials in the q^i and $\dot{q}^i$, then we define

$$\left(\frac{\partial f}{\partial q^i}, h\right) = \lim_{\epsilon \to 0, \epsilon \in \mathbb{R}} \frac{1}{\epsilon}[f(q^1, \ldots q^{i-1}, q^i + \epsilon h(q, \dot{q}), q^{i+1} \ldots q^n, \dot{q}^1, \ldots \dot{q}^n) - f(q^1 \ldots q^n, \dot{q}^1 \ldots \dot{q}^n)].$$

For example,

$$\left(\frac{\partial}{\partial q^2}(q^1 q^2 q^3), h\right) = q^1 h q^3.$$

For any $h \in \mathscr{B}$, the map $f \mapsto (\partial f/\partial q^i, h)$ is a well defined derivation on the free algebra $\mathscr{B}$. However, in quantum mechanics, the algebra of QMO is not free but has canonical commutation relations. If the metric of the configuration space of the quantum-mechanical system is $g_{ij}(q)$ then the commutation relations of the coordinate and velocity observables are

$$[q^i, q^j] = 0, \qquad i, j = 1, \ldots, n \tag{2.1}$$

$$[q^i, \dot{q}^j] - \mathrm{i}g^{ij}(q) = 0, \tag{2.2}$$

$$[\dot{q}^i, \dot{q}^j] - \tfrac{1}{2}\mathrm{i}\{G_k^{ij}(q), \dot{q}^k\} = 0 \tag{2.3}$$

where repeated indices are summed,

$$G_k^{ij} = g^{ia}\Gamma^j_{ak} - g^{ja}\Gamma^i_{ak},$$

Γ is the Christoffel symbol, and the curly brackets are anticommutators.

Strictly speaking, if there is a linear term $A^i(q)p_i$ in the Hamiltonian, then equation (2.3) must be replaced by the equation

$$[\dot{q}^i, \dot{q}^j] - \tfrac{1}{2}\mathrm{i}\{G_k^{ij}, \dot{q}^k\} = \mathrm{i}(A^{i;j} - A^{j;i}), \tag{2.4}$$

where the semicolon denotes covariant differentiation. In this section we shall restrict ourselves to the case $A = 0$ for simplicity of exposition.

By imposing the commutation relations (2.1)–(2.3) we identify certain polynomials, elements of the free algebra $\mathscr{B}$, with zero. We thus form equivalence classes of elements of $\mathscr{B}$ to get a smaller algebra $\mathfrak{A}$ which is mathematically the quotient $\mathscr{B}/\mathscr{I}$ of $\mathscr{B}$ by its two sided ideal $\mathscr{I}$ generated by the polynomials comprising the left-hand sides of equations (2.1)–(2.3) for $i, j = 1, \ldots, n$. The condition for a derivation defined on $\mathscr{B}$ to induce a well defined derivation on the quotient $\mathscr{B}/\mathscr{I}$ is that it annuls $\mathscr{I}$, ie the derivation must annihilate all the left-hand sides of equations (2.1)–(2.3). Such a derivation is said to 'pass to the quotient'. We now consider what variations are required in a formulation of the problem of the calculus of variations, and whether they are well defined derivations on the quotient algebra.

The action integral between times t_0 and t_1 for a Lagrangian $L(q, \dot{q})$ is the integral

$$W_{10} = \int_{t_0}^{t_1} L(q, \dot{q})\,\mathrm{d}t.$$

Suppose that $\epsilon(t)$ is some infinitesimal c-number function of time and $X^i(q(t))$, $i = 1, \ldots, n$ are some functions of the q. In II we considered the variation $\delta_{\epsilon X}L$ in the Lagrangian due to the variations $q^i(t) \to q^i(t) + \epsilon(t)X^i(q(t))$, $\dot{q}^i \to \dot{q}^i + (\epsilon X^i)^{\cdot}$ of the coordinates and velocities. The resulting change in Lagrangian is

$$\delta_{\epsilon X}L = \left(\frac{\partial L}{\partial q^i}, \epsilon X^i\right) + \left(\frac{\partial L}{\partial \dot{q}^i}, (\epsilon X^i)^{\cdot}\right),$$

and we deduced a criterion for $\int_{t_0}^{t_1} \delta_{\epsilon X}L\,\mathrm{d}t$ to vanish for all C^2 functions $\epsilon(t)$ which vanish at the end points t_0, t_1, in the form of the Euler–Lagrange equation

$$\delta_X L = \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}^i}, X^i\right). \tag{2.5}$$

The question arises whether the derivation $\delta_{\epsilon X}$ is well defined on $\mathfrak{A}$. The conditions for this are that

$$0 = \delta_{\epsilon X}([q^i, q^j]), \tag{2.6}$$

$$0 = \delta_{\epsilon X}([q^i, \dot{q}^j] - ig^{ij}(q)) = [q^i, \dot{\epsilon}X^j + \epsilon\dot{X}^j] + [\epsilon X^i, \dot{q}^j] - ig^{ij}{}_{,k}\epsilon X^k$$
$$= i\dot{\epsilon}(X^{i;j} + X^{j;i}), \tag{2.7}$$

$$0 = \delta_{\epsilon X}([\dot{q}^i, \dot{q}^j] - \tfrac{1}{2}i\{G^{ij}_k, \dot{q}^k\}) = i\dot{\epsilon}(X^{i;j} - X^{j;i}) + \tfrac{1}{2}i\epsilon\{H^{ij}_k, \dot{q}^k\} \tag{2.8}$$

where

$$H^{ij}_k = g^{jl}X^i{}_{,kl} - g^{il}X^j{}_{,kl} + X^i{}_{,l}G^{lj}_k - X^j{}_{,l}G^{li}{}_k - X^lG^{ij}{}_{k,l} - X^l{}_{,k}G^{ij}_l$$
$$= \Gamma^j_{ak}(X^{a;i} + X^{i;a}) + g_{ka}(X^{a;i} + X^{i;a})^{;j} - (i \leftrightarrow j).$$

The symbol $(i \leftrightarrow j)$ means that the terms in the same line must be repeated but with i and j interchanged.

Here we have used the fact that equation (2.2) implies that

$$[X^i, \dot{q}^j] = ig^{jk}X^i{}_{,k} \qquad \text{and} \qquad \dot{X}^i = \tfrac{1}{2}\{X^i{}_{,k}, \dot{q}^k\}.$$

The comma denotes partial differentiation.

The equation (2.6) is an identity but equations (2.7) and (2.8) are conditions on X. By setting $\epsilon = 1$ we see that δ_X is a well defined derivation on $\mathfrak{A}$ so long as X obeys the Killing equation for a vector field,

$$X^{i;j} + X^{j;i} = 0. \tag{2.9}$$

However, the equations (2.7) and (2.8) for arbitrary $\epsilon(t)$ imply that X is a parallel vector field, ie

$$X^{i;j} = 0.$$

Now to obtain an Euler–Lagrange equation of motion from a condition of stationary action, $\delta_{\epsilon X}W_{10} = 0$ the function $\epsilon(t)$ must indeed be arbitrary. If $\delta_{\epsilon X}$ is to be a well defined derivation on the algebra $\mathfrak{A}$, we are thus restricted to variations X which are parallel vector fields. Each such allowable variation will lead to one Euler–Lagrange equation of motion. For the action principle to determine the full time-development of the system there need to exist n independent equations of motion and thus n independent parallel vector fields. The only metric which has n independent parallel vector fields is the flat one, $g^{ij} = \delta^{ij}$.

A quick way to see this is to recall the definition (Hicks 1965, p 59) of the curvature tensor R in terms of vector fields, X, Y, Z,

$$R(X, Y)Z = D_XD_YZ - D_YD_XZ - D_{[X,Y]}Z$$

and its property that if f, g, h are scalar fields then

$$R(fX, gY)(hZ) = fghR(X, Y)Z.$$

If $\{e_i\}$, $i = 1, \ldots, n$ are independent parallel vector fields, then

$$D_{e_i}e_j = 0$$

and so

$$R(X, Y)Z = R(X^ie_i, Y^je_j)(Z^ke_k) = X^iY^jZ^kR(e_i, e_j)e_k = 0,$$

that is to say, the curvature tensor vanishes.

The result we have proved is discouraging. It means that one cannot add the left-hand side of equation (2.3) to the Lagrangian and obtain the same Euler–Lagrange equation (2.5) by using the Fréchet derivative unless the variation is a parallel vector field. One can see this directly from the Euler–Lagrange equation by defining the derivation Δ_X on $\mathscr{B}$,

$$\Delta_X f(q, \dot{q}) = \left(\frac{\partial f}{\partial \dot{q}^i}, X^i\right).$$

When $f = L$, this is the quantity which appears in the right-hand side of the Euler–Lagrange equation (2.5). Now

$$\Delta_X([\dot{q}^i, \dot{q}^j] - \tfrac{1}{2}\mathrm{i}\{G^{ij}_k, \dot{q}^k\}) = \mathrm{i}(X^{i;j} - X^{j;i}).$$

Thus the *right-hand* side of equation (2.5) is well defined on $\mathfrak{A}$ only if

$$X^{i;j} - X^{j;i} = 0.$$

This equation, together with the Killing condition (2.9) that the *left-hand* side of equation (2.5) be well defined on $\mathfrak{A}$, tells us that the vector field X must be parallel. In II the difficulty was avoided by just taking the variation to be a Killing vector field and concluding that, in general, we could not add the left-hand side of equation (2.3) to the Lagrangian without changing the Euler–Lagrange equation. In practice, such a restriction presented no serious problems for the Lagrangian under consideration in II since we restricted the Lagrangian to have a symmetric quadratic term. Provided X is Killing, equation (2.2) can be used to modify the Lagrangian without changing the Euler–Lagrange equation and this was the essential requirement in II.

In the rest of this paper we present a modified formulation which avoids these restrictions and has several other advantages. It is coordinate free, so it holds also for systems whose configuration space does not possess a global coordinate system; it makes clear the physical meaning of the operators q^i, $\dot{q}^j$ which we have used somewhat cavalierly in this section, and it provides shorter and more transparent versions of the long-winded formulae which plagued II. The main theme of the modified version is that $\delta_{\epsilon X}$ need not be a *derivation* defined on $\mathfrak{A}$, but only a well defined map, given as a function of the (unique) normal form of each element of $\mathfrak{A}$. The normal form of a general element of $\mathfrak{A}$ is defined in the next section, but in particular the normal forms of the left-hand sides of equations (2.1)–(2.3) are all zero, and so $\delta_{\epsilon X}$ is well-defined on $\mathfrak{A}$ since $\delta_{\epsilon X}(0) = 0$.

3. Quantum mechanics on manifolds

We consider a dynamical system whose configuration space is a C^∞ Riemannian manifold M. We denote by $T^m M$ the space of real valued C^∞ fully symmetric contravariant tensor fields of valence m, for $m = 0, 1, 2, \ldots$. We shall associate with each such tensor $T \in T^m M$ a quantum-mechanical observable $Q(T)$ and postulate commutation relations between these. The direct sum $\oplus_m T^m M$ can be made into a Lie algebra $\mathscr{A}$, where the Lie product of two tensor fields $S^{i_1 \cdots i_m}(q)$, $T^{i_1 \cdots i_n}(q)$ with valences $v(S) = m$, $v(T) = n$ is the symmetric tensor of valence $m+n-1$ given by Sommers (1973):

$$[S, T]^{i_1 \ldots i_{m+n-1}} = m S^{r(i_1 \ldots i_{m-1}} \nabla_r T^{i_m \ldots i_{m+n-1})} - n T^{r(i_1 \ldots i_{n-1}} \nabla_r S^{i_n \ldots i_{n+m-1})}. \tag{3.1}$$

Here the parentheses indicate that the enclosed indices are symmetrized, and the ∇_r

denotes the covariant derivative with respect to the local coordinate q^r. If $S \cap T$ is the tensor of valence $m+n$ which is the symmetrized outer product of tensors S and T then

$$[S, T \cap U] = [S, T] \cap U + T \cap [S, U]. \tag{3.2}$$

The Lie algebra of tensors defined by (3.1) is isomorphic to the Lie algebra of functions on phase space for the following reason. If $p_i = g_{ij}\dot{q}^j$ is the momentum conjugate to q^i and we denote

$$S(q, p) = S^{i_1 \ldots i_m}(q) p_{i_1} \ldots p_{i_m}, \tag{3.3}$$

then the Poisson bracket of $S(q, p)$ and $T(q, p)$ is related to the Lie product $[S, T]$ of the tensor fields S and T by

$$\{S(q, p), T(q, p)\} = -[S, T](q, p). \tag{3.4}$$

We suppose that to each classical function (3.3) on phase space there is a corresponding quantum-mechanical observable $Q(S)$, and that if $c \in \mathbb{R}$,

P1 $\quad Q(S) = 0 \Rightarrow S = 0$

P2 $\quad Q(cS) = cQ(S)$

P3 $\quad Q(S+T) = Q(S)+Q(T)$

P4 $\quad Q(S \cap T) = Q(S)Q(T) \qquad$ if $v(S) = v(T) = 0$

P5 $\quad [Q(S), Q(T)] = -\mathrm{i}Q([S, T]) \qquad$ if $v(S)+v(T) \leqslant 2$

P6 $\quad [Q(g^{-1}), Q(S)] = -\mathrm{i}Q([g^{-1}, S]) \qquad$ for all $S \in \mathscr{A}$.

Here g^{-1} is the inverse of the covariant metric tensor g. The rest of this section is devoted to a discussion of these postulates.

Postulates P1–P6 contain and extend those of Segal (1960). It is not known whether P6 in the case $v(S) > 2$ contradicts P1–P5. The postulates P1–P6 are consistent if $v(S) \leqslant 2$ in P6 and lead to the following results (Bloore and Underhill 1973, Bloore and Routh 1974). If $\phi \in T^0M$, $X, Y \in T^1M$, $S \in T^2M$, then

$$Q(\phi X) \equiv Q(\phi \cap X) = \tfrac{1}{2}\{Q(\phi), Q(X)\}, \tag{3.5}$$

$$Q(X \cap Y) = \tfrac{1}{2}(Q(X) - \tfrac{1}{2}\mathrm{i}Q(\mathrm{div}\, X))(Q(Y) + \tfrac{1}{2}\mathrm{i}Q(\mathrm{div}\, Y)) - \tfrac{1}{8}Q(\Delta(X \cdot Y)) + (X \leftrightarrow Y), \tag{3.6}$$

$$Q(\phi S) \equiv Q(\phi \cap S) = \tfrac{1}{2}\{Q(\phi), Q(S)\} + \tfrac{1}{4}Q(\mathrm{div}[S, \phi] - 2\,\mathrm{grad}\,\phi \,.\, \mathrm{grad}\,\mathrm{Tr}\, S - (\Delta\phi)\,\mathrm{Tr}\, S), \tag{3.7}$$

where Δ is the Laplacian and a dot between two vectors denotes a scalar product. The equation (3.7) follows from (3.5) and (3.6). We have not yet been able to express $Q(X \cap Y \cap Z)$ in terms of $Q(X)$, $Q(Y)$ and $Q(Z)$, in the form analogous to (3.6),

$$Q(X \cap Y \cap Z) = Q(X)Q(Y)Q(Z) + \text{lower-order terms} \tag{3.8}$$

but we conjecture that such an expression exists and is uniquely specified by P1–P6, and that similar expressions hold for all higher tensors,

$$Q\left(\bigcap_{i=1}^{N} X_{(i)}\right) = Q(X_{(1)})Q(X_{(2)}) \ldots Q(X_{(N)}) + \text{lower-order terms.} \tag{3.9}$$

We do not assume (3.9) in this paper, except when $N = 2$, where (3.6) has been proved.

By the algebra of QMO $\mathfrak{A}$ we mean the algebra over the complex numbers $\mathbb{C}$ of polynomials in the $Q(S)$, for all $S \in T^m M$ for all m, with the identifications given by P1–P6. It would be a consequence of (3.9) that any element x of $\mathfrak{A}$ can be uniquely written in 'normal form', $x = x_{\mathrm{R}} + \mathrm{i}x_{\mathrm{I}}$, where

$$x_{\mathrm{R,I}} = \sum_{m=0}^{N} Q(S^{(m)}_{\mathrm{R,I}}) \qquad \text{where} \qquad S^{(m)}_{\mathrm{R,I}} \in T^m M. \tag{3.10}$$

We shall need this result restricted to $N = 2$; that any element x of $\mathfrak{A}$ of the form

$$x = c_1 Q(\phi)Q(T) + c_2 Q(X)Q(Y), \qquad c_i \in \mathbb{C}; \phi \in T^0 M; X, Y \in T^1 M; T \in T^2 M$$

has a unique normal form (3.10) with $N = 2$,

$$x = Q(S^{(0)}_{\mathrm{R}}) + Q(S^{(1)}_{\mathrm{R}}) + Q(S^{(2)}_{\mathrm{R}}) + \mathrm{i}(Q(S^{(0)}_{\mathrm{I}}) + Q(S^{(1)}_{\mathrm{I}}) + Q(S^{(2)}_{\mathrm{I}})).$$

We define the involution * on $\mathfrak{A}$ by

$$(cQ(S))^* = \bar{c}Q(S), \qquad (Q(S)Q(T))^* = Q(T)Q(S)$$

and say x is *Hermitian* if $x = x^*$.

The tensor S is called a Killing tensor if (Sommers 1973)

$$[g^{-1}, S] = 0.$$

If S and T are Killing tensors, so are $S \cap T$ and $[S, T]$, and thus the Killing tensors form a sub-algebra $\mathscr{K}$ of $\mathscr{A}$. In the absence of a potential the classical Hamiltonian is $\frac{1}{2}g^{ij}(q)p_i p_j$ or $\frac{1}{2}g^{-1}(q, p)$ in the notation of equation (3.3). Hamilton's equations imply that

$$\frac{\mathrm{d}}{\mathrm{d}t}S(q, p) = \{S(q, p), \tfrac{1}{2}g^{-1}(q, p)\} = -[S, \tfrac{1}{2}g^{-1}](q, p)$$

so that Killing tensors correspond in classical mechanics to constants of the free motion.

We suppose that the commutation relations P5 and P6 are equal-time commutation relations and that the time development of the observables is according to the equation

$$\frac{\mathrm{d}}{\mathrm{d}t}Q(S) = \mathrm{i}[Q(H), Q(S)] = Q([H, S]), \tag{3.11}$$

where

$$H = \tfrac{1}{2}g^{-1} + A + V$$

and A and V are prescribed vector and scalar fields. Evidently $Q(S)$ is a conserved QMO of the free motion ($A = V = 0$) whenever S is Killing. As a particular case of (3.11) we note that for any scalar field ϕ,

$$\frac{\mathrm{d}}{\mathrm{d}t}Q(\phi) = Q(\mathrm{grad}\ \phi) + Q(A\phi). \tag{3.12}$$

If we assume that the manifold M admits a global coordinate system $q^1, \ldots, q^n$, then the coordinates q^i are scalar fields on M and give basic vector fields $e_i = g_{ij}\,\mathrm{grad}\, q^j$. The coordinate observables are $Q(q^i)$ and the corresponding conjugate momentum observables are $Q(e_i)$. The postulate P5 gives the commutation relations

$$[Q(q^i), Q(q^j)] = [Q(e_i), Q(e_j)] = 0, \qquad [Q(e_i), Q(q^j)] = -\mathrm{i}\delta^j_i.$$

Using equations (3.5) and (3.12) we may write

$$\frac{\mathrm{d}}{\mathrm{d}t}Q(q^i) = \tfrac{1}{2}\{Q(g^{ij}), Q(e_j)\} + Q(A^i)$$

and obtain the commutation relations (2.1), (2.2) and (2.3) for the coordinate and velocity observables.

The postulate P5 cannot be strengthened to hold for all S, T without violating the other postulates. If, however, X is a Killing vector and S has valence 2 or less, then (Bloore and Routh 1974)

$$[Q(X), Q(S)] = -\mathrm{i}Q([X, S]). \tag{3.13}$$

We conjecture that equation (3.13) will hold for tensors S of all valences so long as X is Killing but this cannot be proved until we have an explicit form for $Q(X \cap Y \cap Z)$.

The result (3.13) enables us to relate inner derivations on $\mathscr{A}$ and on $\mathfrak{A}$. For any vector field X on the manifold M, the mapping from $\mathscr{A}$ to $\mathscr{A}$

$$S \mapsto [X, S] \equiv \delta_X S$$

is an (inner) derivation on $\mathscr{A}$. Also the mapping from $\mathfrak{A}$ to $\mathfrak{A}$

$$Q(S) \mapsto \mathrm{i}[Q(X), Q(S)] \equiv \delta_X Q(S) \tag{3.14}$$

is an inner derivation on $\mathfrak{A}$.

If $v(S) \leqslant 1$ then by P5,

$$\delta_X Q(S) = Q(\delta_X S). \tag{3.15}$$

The equation (3.15) extends to $v(S) = 2$ so long as X is Killing.

4. Lagrangian quantum theory

In this section we pose and solve the same problem as the second paper in this series, but in the coordinate-free formalism developed in § 3. We consider a quantum-mechanical system which has a C^∞ Riemannian configuration manifold M with metric tensor g. We suppose that the quantum-mechanical observables obey postulates P1–P6, with the time dependence generated by the quantum Hamiltonian:

$$Q(H) = Q(\tfrac{1}{2}g^{-1}) + Q(A) + Q(V), \qquad A \in T^1M, V \in T^0M \tag{4.1}$$

that is,

$$\frac{\mathrm{d}}{\mathrm{d}t}Q(S) = \mathrm{i}[Q(H), Q(S)]. \tag{4.2}$$

We seek a (quadratic) quantum-mechanical Lagrangian, which will thus have the normal form

$$Q(L) = Q(L^{(2)}) + Q(L^{(1)}) + Q(L^{(0)})$$

where $L^{(i)} \in T^iM$, and also a class of vector fields $\{X\}$, which satisfy Hamilton's principle of stationary action. That is to say, the quantum-mechanical action

$$Q(W_{10}) = \int_{t_0}^{t_1} Q(L)\,\mathrm{d}t \tag{4.3}$$

is stationary with respect to variations of the form

$$Q(L) \to Q(L) + \hat{\delta}_{\epsilon X} Q(L) \tag{4.4}$$

where $\epsilon(t)$ is an arbitrary real C^2 function of t which vanishes at t_0 and t_1. The variation $\hat{\delta}_{\epsilon X}$ is defined as follows:

$$\hat{\delta}_{\epsilon X} Q(L^{(0)}) = \epsilon Q(\delta_X L^{(0)}), \tag{4.5}$$

$$\hat{\delta}_{\epsilon X} Q(L^{(1)}) = \epsilon Q(\delta_X L^{(1)} + \tilde{X} \,.\, L^{(1)} - [X, A] \,.\, L^{(1)}) + \dot{\epsilon} Q(X \,.\, L^{(1)}), \tag{4.6}$$

$$\hat{\delta}_{\epsilon X} Q(L^{(2)}) = \epsilon Q(\delta_X L^{(2)} + \tilde{X} \,.\, L^{(2)} + L^{(2)} \,.\, \tilde{X} - 2[X, A] \,.\, L^{(2)}) + 2\dot{\epsilon} Q(X \,.\, L^{(2)}), \tag{4.7}$$

where

$$\tilde{X} = [g^{-1}, X], \qquad (\tilde{X} \,.\, L^{(2)})^{ij} = \tilde{X}^{ik} L^{(2)}{}_k{}^j.$$

The curious right-hand sides of equations (4.5)–(4.7) are suggested by the coordinate-free versions of the variations used in classical mechanics. For example, the QMO $Q(L^{(2)})$ corresponds to the classical function $L^{(2)ij}(q)p_i p_j$ which becomes

$$\Lambda(q, \dot{q}) = L^{(2)}{}_{ij}(q)(\dot{q}^i - A^i)(\dot{q}^j - A^j)$$

when written in terms of velocities rather than momenta, as is required in the Lagrangian formulation. (The classical Hamiltonian which corresponds to (4.1) is

$$H(q, p) = \tfrac{1}{2} g^{ij}(q) p_i p_j + A^i(q) p_i + V(q) \tag{4.8}$$

so that

$$\dot{q}^i = \frac{\partial H}{\partial p_i} = g^{ij} p_j + A^i.) \tag{4.9}$$

Under the variation

$$q^i \to q^i + \epsilon X^i, \qquad \dot{q}^i \to \dot{q}^i + (\epsilon X^i)^{\cdot}$$

which is used in classical Lagrangian mechanics, the change in Λ is

$$\begin{aligned}
&\epsilon X^k L_{ij,k}(\dot{q}^i - A^i)(\dot{q}^j - A^j) - 2\epsilon X^k L_{ij} A^i{}_{,k}(\dot{q}^j - A^j) + 2L_{ij}(\dot{\epsilon} X^i + \epsilon \dot{X}^i)(\dot{q}^j - A^j) \\
&\quad = \epsilon([X, L^{(2)}] + \tilde{X} \,.\, L^{(2)} + L^{(2)} \,.\, \tilde{X})_{ij}(\dot{q}^i - A^i)(\dot{q}^j - A^j) \\
&\qquad - 2\epsilon([X, A] \,.\, L^{(2)})_j(\dot{q}^j - A^j) + 2\dot{\epsilon}(X \,.\, L^{(2)})_j(\dot{q}^j - A^j) \\
&\quad = \epsilon([X, L^{(2)}] + \tilde{X} \,.\, L^{(2)} + L^{(2)} \,.\, \tilde{X})^{ij} p_i p_j \\
&\qquad - 2\epsilon([X, A] \,.\, L^{(2)})^j p_j + 2\dot{\epsilon}(X \,.\, L^{(2)})^j p_j.
\end{aligned} \tag{4.10}$$

The right-hand side of (4.7) is the QMO which corresponds to (4.10). The equations (4.5) and (4.6) follow from the form of the classical variations in the same way.

Having justified the covariant forms (4.5), (4.6), (4.7) for the variations we proceed to the problem of finding tensors $L^{(2)}$, $L^{(1)}$, $L^{(0)}$ such that the action (4.3) is stationary with respect to the variations (4.4).

We have

$$0 = \int_{t_0}^{t_1} \hat{\delta}_{\epsilon X}(Q(L^{(2)}) + Q(L^{(1)}) + Q(L^{(0)}))\,\mathrm{d}t$$

$$= \int_{t_0}^{t_1} \{\epsilon Q(N) + \dot{\epsilon} Q(X\,.\,(2L^{(2)} + L^{(1)}))\}\,\mathrm{d}t$$

$$= \int_{t_0}^{t_1} \epsilon \left\{Q(N) - \frac{\mathrm{d}}{\mathrm{d}t} Q(X\,.\,(2L^{(2)} + L^{(1)}))\right\}\mathrm{d}t$$

$$+ \int_{t_0}^{t_1} \frac{\mathrm{d}}{\mathrm{d}t}\{\epsilon Q(X\,.\,(2L^{(2)} + L^{(1)}))\}\,\mathrm{d}t \tag{4.11}$$

where

$$N = [X, L^{(2)} + L^{(1)} + L^{(0)}] + \tilde{X}\,.\,L^{(2)} + L^{(2)}\,.\,\tilde{X} + \tilde{X}\,.\,L^{(1)} - [X, A]\,.\,(2L^{(2)} + L^{(1)}).$$

The second term on the right-hand side of (4.11) vanishes since it is the value of the quantity in braces at the limits, and this is zero because $\epsilon(t_0) = \epsilon(t_1) = 0$. The first term vanishes for all functions $\epsilon(t)$ provided that

$$Q(N) = \frac{\mathrm{d}}{\mathrm{d}t} Q(X\,.\,(2L^{(2)} + L^{(1)})). \tag{4.12}$$

This is the Euler–Lagrange equation for the problem. The time derivative on the right-hand side of equation (4.12) is given by equation (4.2), from which we conclude

$$Q(N) = Q([\tfrac{1}{2}g^{-1} + A + V, X\,.\,(2L^{(2)} + L^{(1)})]). \tag{4.13}$$

Using postulate P1 we drop the Q symbols in equation (4.13) and obtain an equation between the tensor fields themselves. Equating tensors of equal valence we obtain

$$(v = 2) \qquad [g^{-1}, X\,.\,L^{(2)}] = [X, L^{(2)}] + \tilde{X}\,.\,L^{(2)} + L^{(2)}\,.\,\tilde{X} \tag{4.14}$$

$$(v = 1) \qquad [A, X\,.\,2L^{(2)}] + [\tfrac{1}{2}g^{-1}, X\,.\,L^{(1)}] = [X, L^{(1)}] - [X, A]\,.\,2L^{(2)} + \tilde{X}\,.\,L^{(1)} \tag{4.15}$$

$$(v = 0) \qquad [A, X\,.\,L^{(1)}] + [V, 2X\,.\,L^{(2)}] = [X, L^{(0)}] - [X, A]\,.\,L^{(1)}. \tag{4.16}$$

The equations (4.14)–(4.16) are the conditions on the tensor fields $L^{(0)}$, $L^{(1)}$, $L^{(2)}$ which appear in the Lagrangian and on the vector field X which ensure that the action (4.3) is stationary for the variations (4.4) given by (4.5)–(4.7). It remains to find a solution of these equations.

The equation (4.14) in coordinates reduces to

$$X_m(L^{(2)mi;j} + L^{(2)mj;i} - L^{(2)ij;m}) = 0. \tag{4.17}$$

We suppose that sufficient allowable variations X exist to span the tangent space at each point of the configuration manifold M. Then equation (4.17) implies that

$$L^{(2)mi;j} + L^{(2)mj;i} - L^{(2)ij;m} = 0.$$

Interchanging m and i in this equation and adding the results gives

$$L^{(2)mi;j} = 0$$

and thus for indecomposable manifolds (Eisenhart 1923)

$$L^{(2)} = \tfrac{1}{2}\lambda g^{-1}$$

where λ is a constant. Substitution of this result into equation (4.15) yields

$$X \cdot (\nabla \times L^{(1)}) = 0$$

whence

$$\nabla \times L^{(1)} = 0.$$

Let us next suppose that M is simply connected. Then $L^{(1)}$ is the gradient of some scalar field ϕ on M and

$$Q(L^{(1)}) = Q(\text{grad } \phi) = \frac{\mathrm{d}}{\mathrm{d}t} Q(\phi) - Q(A\phi).$$

The equation (4.16) now becomes

$$[X, L^{(0)} + \lambda V - A\phi] = 0$$

which implies

$$L^{(0)} = -\lambda V + A\phi.$$

Thus, for an indecomposable simply-connected manifold and the time development given by the Hamiltonian (4.1) the quantum-mechanical Lagrangian has the form

$$Q(L) = \lambda Q(\tfrac{1}{2}g^{-1} - V) + \frac{\mathrm{d}}{\mathrm{d}t} Q(\phi)$$

where ϕ is an arbitrary scalar field. The allowable variations for which the action integral of this Lagrangian are stationary are those given by equations (4.5)–(4.7) where the vector field X is quite arbitrary.

Acknowledgments

LR thanks the Science Research Council for a studentship.

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