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Lagrangian quantum theory IV. Schouten concomitants and the Dirac problem

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Abstract. We formulate Hamilton's principle of stationary action in classical mechanics using the Lie algebra of Schouten concomitants of symmetric contravariant tensor fields on the configuration space of the system. Such a formulation is global and coordinate free. We show that a directly parallel formulation holds in quantum mechanics so long as all the Poisson brackets involved can be replaced in the quantum version by commutators in a canonical way. We discuss an example (where the Hamiltonian possesses a velocity-dependent potential) in which this cannot be done, and conclude that in this case the action is stationary only for a subclass of variations, namely those corresponding to Killing vector fields on the configuration manifold.

1. Introduction

This paper continues the series (Bloore *et al* 1973, Bloore and Routh 1973, 1974a) on the formulation of a Hamiltonian principle of stationary action for (holonomic) quantum-mechanical systems with a finite number of degrees of freedom. In the previous paper of the series (Bloore and Routh 1974a) we formulated such a principle in the case when the term in the Hamiltonian which was quadratic in the momentum had the form $\frac{1}{2}g^{ij}(q)p_ip_j$ where g_{ij} is the metric tensor of the (Riemannian) configuration space M of the system. That work is shown here to rest heavily on the fact that all the commutators which were needed were in a sense 'canonical'. That is to say, all Poisson brackets which were used in the classical theory became commutator brackets in the quantized version. Now it is well known (and discussed in connection with the present theory by Bloore and Routh (1974b)) that it is not possible to arrange for *all* commutators to be canonical. (The problem of making quantum-mechanical quantities from classical ones such that Poisson brackets turn into commutator brackets is called the Dirac problem.) We shall exhibit a Hamiltonian which is sometimes used in nuclear physics (one with a quadratic term $\frac{1}{2}(h^{-1}(q))^{ij}p_ip_j$ with $h \neq g$, corresponding to a 'velocity-dependent potential' (Kiang *et al* 1969)) for which the corresponding action cannot be stationary for all variations of the class obtained in paper III, but only for some, namely those which correspond to Killing vector fields on the configuration manifold. We show that this restriction results from the fact that the commutator of this Hamiltonian with the momentum along a vector field X is non-canonical unless X is Killing.

In § 2 we present the passage from classical Hamiltonian mechanics to classical Lagrangian mechanics using the Lie algebra $\mathscr{A}$ of symmetric contravariant tensor fields

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which has the Schouten bilinear concomitant as Lie product. To each vector field X on the configuration manifold M of the system we define an associated 'variation' $\delta_{\epsilon X}$ of the tensor fields in $\mathscr{A}$. This map $\delta_{\epsilon X}$ is actually a map defined on the enveloping algebra of $\mathscr{A}$ and is equivalent to the usual variation employed in classical Lagrangian mechanics. We obtain the Euler–Lagrange equation from the condition that the action

$$\int_{t_0}^{t_1} L \, \mathrm{d}t \tag{1.1}$$

be stationary for the variation $\delta_{\epsilon X}$. Although this equation involves X, we show that for a time development prescribed by a given arbitrary quadratic Hamiltonian, we can 'solve' the Euler–Lagrange equation to find the Lagrangian in terms of the Hamiltonian in such a way that the equation is satisfied for all variations $\delta_{\epsilon X}$. Hence the action defined by this Lagrangian is stationary for all $\delta_{\epsilon X}$.

This formulation of classical mechanics, being global and coordinate independent, allows the straightforward transposition into quantum mechanics which was made in paper III for the case $h = g$. We show here that the Euler–Lagrange equation can be solved for the Lagrangian in the quantum-mechanical case in such a way that it holds for all variations $\delta_{\epsilon X}$ only if the Schouten concomitants are related to the commutator brackets in the canonical way. Whereas this is indeed the case when $h = g$, it is not the case otherwise. If $h \neq g$, it is only possible to satisfy the Euler–Lagrange equation for variations which correspond to Killing vector fields, since the commutator of the quantum-mechanical observables which correspond to the classical functions $(h^{-1}(q))^{ij}p_ip_j$ and $X^i(q)p_i$ are canonical for all second-order tensors $h^{-1}(q)$ only if X is Killing.

2. Classical mechanics using concomitants

We wish to describe the transformation from the Hamiltonian to the Lagrangian formulation of classical mechanics using the Schouten concomitant algebra of symmetric contravariant tensor fields. (See Sommers (1973) and references cited there.) Let S be such a tensor field of valence m, given in some coordinate patch on M by components $S^{i_1 \dots i_m}(q^1, \dots, q^n)$. Denote the homogeneous function of order m in momentum

$$S^{i_1 \dots i_m}(q)p_{i_1} \dots p_{i_m} \equiv C(S), \tag{2.1}$$

and denote $T^{(m)}M$ the space of all such tensor fields S on M. If $U \in T^{(n)}M$, then the Schouten concomitant $[S, U]$ is the tensor of order $m+n-1$ given by

$$[S, U]^{i_1 \dots i_{m+n-1}} = mS^{r(i_1 \dots i_{m-1}}\partial_r U^{i_m \dots i_{m+n-1})} - nU^{r(i_1 \dots i_{n-1}}\partial_r S^{i_n \dots i_{n+m-1})} \tag{2.2}$$

where the round brackets indicate symmetrization of the enclosed indices. The concomitant is related to the Poisson bracket by

$$\{C(S), C(U)\} = -C([S, U]). \tag{2.3}$$

We shall make a convenient abuse of notation by writing $C(S)+C(U)$ as $C(S+U)$, even when S and U have different valence.

We shall suppose that the Hamiltonian is

$$H(q, p) = C(\tfrac{1}{2}h^{-1} + A + V) \tag{2.4}$$

where $h^{-1} \in T^{(2)}M$, $A \in T^{(1)}M$, $V \in T^{(0)}M$. The equation of motion is then

$$\frac{\mathrm{d}}{\mathrm{d}t}C(S) = C([\tfrac{1}{2}h^{-1}+A+V, S]). \tag{2.5}$$

In order to develop the Lagrangian formulation of classical mechanics in terms of the Schouten algebra we must first express in these terms the variation $\delta_{\epsilon X}C(S)$ of $C(S)$ which arises when we make the usual Lagrangian variations of coordinates and velocities

$$q^i(t) \to q^i(t)+\epsilon(t)X^i(q(t)), \qquad \dot{q}^i \to \dot{q}^i+(\epsilon X^i(q))^{\cdot}, \tag{2.6}$$

in the action integral (1.1). Here $\epsilon(t)$ is an arbitrary real C^2 function of time which vanishes at t_0 and t_1, and X is an arbitrary vector field on M. In view of equation (2.1), we must first express the momenta p_i in terms of the velocities $\dot{q}^j$. By equation (2.5),

$$\dot{q}^i = \frac{\partial H}{\partial p_i} = (h^{-1})^{ij}p_j + A^i \tag{2.7}$$

so that

$$p_i = h_{ij}(\dot{q}^j - A^j). \tag{2.8}$$

We do not assume that h is the metric tensor g which raises and lowers suffices. Thus

$$(h^{-1})_{ij} \equiv g_{il}g_{jm}(h^{-1})^{lm}$$

differs from h_{ij}.

If the valence $v(S) = 0$, S is a scalar field on M and $S = C(S)$ and

$$\delta_{\epsilon X}C(S) = \frac{\partial S}{\partial q^k}\epsilon X^k = \epsilon C([X, S]). \tag{2.9}$$

If $v(S) = 1$, then, denoting $X^i{}_{.k} \equiv \partial X^i/\partial q^k$,

$$C(S) = S^i(q)p_i = S^i(q)h_{ij}(q)(\dot{q}^j - A^j(q))$$

and

$$\begin{aligned}\delta_{\epsilon X}C(S) &= \epsilon X^k\frac{\partial}{\partial q^k}C(S)+(\dot{\epsilon}X^k+\epsilon\dot{X}^k)\frac{\partial}{\partial \dot{q}^k}C(S) \\ &= \epsilon C([X, S]+S \lrcorner h \llcorner [h^{-1}, X]+S \lrcorner h \llcorner [A, X])+\dot{\epsilon}C(X \lrcorner h \llcorner S)\end{aligned} \tag{2.10}$$

where $X \lrcorner h \llcorner S$ is the scalar field $X^a h_{ab} S^b$. Similarly one finds that if $v(S) = 2$ then

$$\begin{aligned}\delta_{\epsilon X}C(S) = {}& \epsilon C([X, S]+[h^{-1}, X] \lrcorner h \llcorner S+S \lrcorner h \llcorner [h^{-1}, X]+2S \lrcorner h \llcorner [A, X]) \\ &+2\dot{\epsilon}C(X \lrcorner h \llcorner S).\end{aligned} \tag{2.11}$$

Let us suppose that the quantities $C(S)$ vary with time according to equations (2.5). Given this time dependence, we now pose the problem: find a Lagrangian

$$L = C(L^{(2)}+L^{(1)}+L^{(0)}) \tag{2.12}$$

where $L^{(i)} \in T^{(i)}M$ such that the action integral (1.1) is stationary with respect to the variations (2.6), which are equivalent to the variations $\delta_{\epsilon X}$ defined in equations (2.9–11).

The argument proceeds exactly as in § 4 of paper III except that the symbol Q there is replaced by the symbol C. We obtain the Euler–Lagrange equation

$$C(N) = \frac{\mathrm{d}}{\mathrm{d}t} C(X \lrcorner h \llcorner (2L^{(2)} + L^{(1)})) \tag{2.13}$$

where

$$\begin{aligned} N = {} & [X, L^{(2)} + L^{(1)} + L^{(0)}] + [h^{-1}, X] \lrcorner h \llcorner L^{(2)} + L^{(2)} \lrcorner h \llcorner [h^{-1}, X] + L^{(1)} \lrcorner h \llcorner [h^{-1}, X] \\ & + (2L^{(2)} + L^{(1)}) \lrcorner h \llcorner [A, X]. \end{aligned} \tag{2.14}$$

The right-hand side of equation (2.13) is given by the Hamilton equation of motion (2.5), so that using (2.3) we may write

$$C(N) = C([\tfrac{1}{2}h^{-1} + A + V, X \lrcorner h \llcorner (2L^{(2)} + L^{(1)})]). \tag{2.15}$$

Dropping the symbols C and equating tensors of equal valence in equation (2.15) we obtain

$$[X, L^{(2)}] + [h^{-1}, X] \lrcorner h \llcorner L^{(2)} + L^{(2)} \lrcorner h \llcorner [h^{-1}, X] = [\tfrac{1}{2}h^{-1}, X \lrcorner h \llcorner 2L^{(2)}] \tag{2.16}$$

$$\begin{aligned} & [X, L^{(1)}] + L^{(1)} \lrcorner h \llcorner [h^{-1}, X] + 2L^{(2)} \lrcorner h \llcorner [A, X] \\ & \qquad = [\tfrac{1}{2}h^{-1}, X \lrcorner h \llcorner L^{(1)}] + [A, X \lrcorner h \llcorner 2L^{(2)}] \end{aligned} \tag{2.17}$$

$$[X, L^{(0)}] + L^{(1)} \lrcorner h \llcorner [A, X] = [A, X \lrcorner h \llcorner L^{(1)}] + [V, X \lrcorner h \llcorner 2L^{(2)}]. \tag{2.18}$$

The equations (2.16) and (2.17) do not depend on the metric g. We may re-express the equation (2.16) as

$$X_m(L^{(2)mi:j} + L^{(2)mj:i} - L^{(2)ij:m}) = 0 \tag{2.19}$$

where the suffices are raised and lowered with respect to the tensor field h regarded as a metric and the colon denotes covariant differentiations with respect to the metric h. We suppose that sufficient allowable variations X exist to span the tangent space at each point of the configuration manifold so that equation (2.19) implies

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

and thus (by interchanging m and i in this equation and adding the results)

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

We shall suppose that h is an indecomposable tensor on M; it then follows from a theorem of Eisenhart (1923) that

$$L^{(2)} = \tfrac{1}{2}\lambda h^{-1} \tag{2.20}$$

where λ is a constant. Substitution of this result into equation (2.17) yields

$$X_m(\nabla \wedge L^{(1)})^{mn} = 0$$

whence

$$\nabla \wedge L^{(1)} = 0 \tag{2.21}$$

where X_m stands for $h_{ma}X^a$ and ∇ denotes covariant differentiation with respect to the metric h. We next suppose that the configuration manifold M is simply connected.

Then equation (2.21) implies that $L^{(1)}$ is the h-gradient of some scalar field ϕ,

$$C(L^{(1)}) = C([\tfrac{1}{2}h^{-1}, \phi]) = \frac{\mathrm{d}}{\mathrm{d}t}C(\phi) - C(A\phi). \tag{2.22}$$

The equation (2.18) now reduces to

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

so that

$$L^{(0)} = -\lambda V + A\phi. \tag{2.23}$$

Thus for the motion governed by the Hamiltonian (2.4), the most general Lagrangian which obeys the Euler–Lagrange equation (2.13) for all vector fields X is

$$L = \lambda C(\tfrac{1}{2}h^{-1} - V) + \frac{\mathrm{d}}{\mathrm{d}t}C(\phi) \tag{2.24}$$

where ϕ is an arbitrary scalar field and λ is an arbitrary constant.

3. Transition to quantum mechanics

In paper III we introduced the algebra $\mathfrak{A}$ of quantum-mechanical observables (QMO) $Q(S)$. To each function $C(S)$ defined in the previous section on classical phase space, we introduced the corresponding QMO $Q(S)$, and postulated the equal-time commutation relations

$$[Q(S), Q(U)] = -\mathrm{i}Q([S, U]) \qquad \text{if } v(S) + v(U) \leqslant 2 \tag{3.1}$$

$$[Q(g^{-1}), Q(S)] = -\mathrm{i}Q([g^{-1}, S]) \qquad \text{if } v(S) = 1. \tag{3.2}$$

The equation (3.1) is canonical in the sense that the commutator of the QMO of $C(S)$ and $C(U)$ is equal to i times the QMO of the Poisson bracket

$$\{C(S), C(U)\} = -C([S, U]).$$

Unfortunately, this rule cannot be extended to tensors S, U of arbitrary valence. In particular we have shown (Bloore and Routh 1974b) that equations (3.1) and (3.2) imply that for $v(h^{-1}) = 2$, $v(X) = 1$,

$$\begin{aligned}
[Q(h^{-1}), Q(X)] &= -\mathrm{i}Q([h^{-1}, X]) + \frac{\mathrm{i}}{4}Q(\operatorname{div}[h^{-1}, \operatorname{div} X] - \Delta \operatorname{Tr}[h^{-1}, X] - [X, \Delta \operatorname{Tr} h^{-1}]) \\
&= -\mathrm{i}Q([h^{-1}, X]) + \frac{\mathrm{i}}{8}Q(\operatorname{div}[h^{-1}, \operatorname{Tr} \tilde{X}] - 2\Delta \operatorname{Tr}(h^{-1} \lrcorner g \llcorner \tilde{X}) \\
&\quad + 2 \operatorname{div}[\tilde{X}, \operatorname{Tr} h^{-1}] - [[\tfrac{1}{2}g^{-1}, \operatorname{Tr} \tilde{X}], \operatorname{Tr} h^{-1}]) \\
&\equiv -\mathrm{i}(Q([h^{-1}, X]) + Q(\operatorname{Rem}(h^{-1}, \tilde{X}))).
\end{aligned} \tag{3.3}$$

Here $\tilde{X}$ denotes the second-order tensor field $[g^{-1}, X]$ and the second line of equation (3.3) may be obtained from the first by use of the symmetry of the Ricci tensor. Note that the scalar field $\operatorname{Rem}(g^{-1}, \tilde{X})$ vanishes for all X so that equation (3.3) indeed reduces to the canonical equation (3.2).

We now consider a quantum-mechanical system whose time development is given by the Heisenberg equation of motion

$$\frac{\mathrm{d}}{\mathrm{d}t}Q(S) = \mathrm{i}[Q(H), Q(S)] \tag{3.4}$$

where

$$Q(H) = Q(\tfrac{1}{2}h^{-1}+A+V) \tag{3.5}$$

and A, V are prescribed vector and scalar fields on the configuration manifold M of the system. As in paper III, to each vector field X on M we define a 'variation' $\hat{\delta}_{\epsilon X}$ on $\mathfrak{A}$ which is the same as the variation $\delta_{\epsilon X}$ given by equations (2.9–11) but with C replaced by Q. In paper III we treated the usual case $h = g$. We shall show here that, if $h \neq g$, the non-canonical nature of the commutation relation (3.3) prevents the construction of a Lagrangian whose action is stationary with respect to all variations $\hat{\delta}_{\epsilon X}$.

As in paper III we seek a (quadratic) quantum-mechanical Lagrangian

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

whose action is stationary for the variations $\hat{\delta}_{\epsilon X}$:

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

We are led to the Euler–Lagrange equation analogous to equation (2.13),

$$Q(N) = \frac{\mathrm{d}}{\mathrm{d}t}Q(X \lrcorner h \llcorner (2L^{(2)}+L^{(1)})) \tag{3.6}$$

with N given by equation (2.14). The right-hand side of equation (3.6) is given by (3.4) and (3.5) so that

$$\begin{aligned} Q(N) &= \mathrm{i}[Q(\tfrac{1}{2}h^{-1}+A+V), Q(X \lrcorner h \llcorner (2L^{(2)}+L^{(1)}))] \\ &= Q([\tfrac{1}{2}h^{-1}+A+V, X \lrcorner h \llcorner (2L^{(2)}+L^{(1)})]) + Q(\mathrm{Rem}(\tfrac{1}{2}h^{-1}, (X \lrcorner h \llcorner 2L^{(2)})^{\sim})) \end{aligned} \tag{3.7}$$

where we have used equations (3.3) in the second line. Dropping the symbols Q and equating tensors of equal valence in equation (3.7) gives again the equations (2.16) and (2.17) but equation (2.18) has the extra term $\mathrm{Rem}(\tfrac{1}{2}h^{-1}, (X \lrcorner h \llcorner 2L^{(2)})^{\sim})$ on the right-hand side. The equations (2.16) and (2.17) imply as before that

$$L^{(2)} = \tfrac{1}{2}\lambda h^{-1}, \qquad L^{(1)} = [\tfrac{1}{2}h^{-1}, \phi]$$

and then equation (2.18) reduces to

$$[X, L^{(0)} - A\phi + \lambda V] = \lambda\,\mathrm{Rem}(\tfrac{1}{2}h^{-1}, \tilde{X}). \tag{3.8}$$

We regard equation (3.8) as an equation for $L^{(0)}$ in terms of the fields h^{-1}, A, V which appear in the Hamiltonian. We would like the vector field X which characterizes the variation to be as arbitrary as possible. For a general tensor field h^{-1}, the right-hand side of equation (3.8) cannot be cast in the form $[X, \psi]$ where ψ is a scalar field. The class of allowable variations X which is common to all choices of h^{-1} in the Hamiltonian is the class for which $\tilde{X}$ vanishes, that is the variations corresponding to Killing vector fields. The solution of equation (3.8) for $L^{(0)}$ is then equation (2.23) and the Lagrangian is (2.24) with C replaced by Q. In the case $h = g$ discussed in paper III, $\mathrm{Rem}(\tfrac{1}{2}g^{-1}, \tilde{X})$

vanishes for all X as noted before, so that all vector fields are then allowable and not just the Killing ones.

One might perhaps argue that one can make the equation (3.3) canonical by *fiat* in the case when the Hamiltonian is (3.5), simply by taking the canonical commutation relation (3.2) to hold for h^{-1} rather than for g^{-1}. The overwhelming argument against this is that equal-time commutation relations of coordinates with momenta are kinematical in nature and should not depend on the choice of the velocity dependent potential which is applied but only on the characteristics of the configuration manifold of the system.

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