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The Action Principle in Quantum Mechanics

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Abstract

The Euler–Lagrange equation derived from Schwinger's action principle (1951) has been shown by Kiang *et al.* (1969) and Lin *et al.* (1970) to lead to inconsistencies for quadratic lagrangians of the form

$$\bar{L}(\dot{q}, q) = \tfrac{1}{2}\dot{q}^j g_{jk}(q)\dot{q}^k - V(q)$$

except in the Euclidean case $g_{jk} = \delta_{jk}$. This inadequacy is linked to Schwinger's specification that the variations of operators be *c*-numbers. We reformulate the action principle by introducing the concept of 'proper' Gauteaux variation of operators to find the most general class of admissible variation consistent with the postulated quantisation rules. This new action principle, applied to the Lagrangian $\bar{L}$, yields a quantum Euler equation consistent with the Hamilton–Heisenberg equations.

1. *Introduction*

Various types of classical variational principles‡ (V.P.) have been designed since the 'principle of least action' was put forward by Maupertuis (1744) two centuries ago. However, by far the most important V.P. are the two formulated mainly by Hamilton (1834, 1835). In the traditional coordinate notation where $\dot{q}^k = (d/dt)q^k$, the principle involves the action integrals

$$\mathscr{A}(\dot{q}, q) = \int_{t'}^{t''} L(\dot{q}, q, t) \tag{1.1}$$

and

$$\mathscr{M}\mathscr{A}(q, p) = \int_{t'}^{t''} (p_k\dot{q}^k - H(q, p, t))\, dt \tag{1.2}$$

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‡ For discussion on various principles in Physics see Yourgrau & Mandelstram (1972).

What is commonly referred to a Hamilton action principle† is precisely specified by

$$\delta\mathscr{A}(\dot{q}, q; \delta\dot{q}, \delta q) = 0 \tag{1.3}$$

where $\delta\mathscr{A}$ is the Gauteaux variation ‡ which is the limit, as $\epsilon \to 0$, of

$$\epsilon^{-1}(\mathscr{A}(\dot{\mathbf{q}} + \epsilon\delta\dot{\mathbf{q}}, \mathbf{q} + \epsilon\delta\mathbf{q}) - \mathscr{A}(\dot{\mathbf{q}}, \mathbf{q}))$$

the variations $\delta\dot{\mathbf{q}}$ and $\delta\mathbf{q}$ being classically constrained by

$$\delta\dot{\mathbf{q}} = (d/dt)\,\delta\mathbf{q} \tag{1.4}$$

and

$$\delta\mathbf{q}(t') = \delta\mathbf{q}(t'') = 0 \tag{1.5}$$

This V.P. yields the Euler–Lagrange equation

$$\frac{d}{dt}\frac{\partial L}{\partial\dot{q}^k} - \frac{\partial L}{\partial q^k} = 0, \qquad k = 1, \ldots, N \qquad \text{(Classical)} \tag{1.6}$$

On the other hand the specification that

$$\delta\mathscr{M}\mathscr{A}(\mathbf{q}, \mathbf{p}; \delta\mathbf{q}, \delta\mathbf{p}) = \lim_{\epsilon\to 0}\frac{\mathscr{M}\mathscr{A}(\mathbf{q} + \epsilon\,\delta\mathbf{q}, \mathbf{p} + \epsilon\,\delta\mathbf{p}) - \mathscr{M}\mathscr{A}(\mathbf{q}, \mathbf{p})}{\epsilon}$$
$$= 0 \tag{1.7}$$

subject to the vanishing of the variations at the end-points

$$\delta\mathbf{q}(t') = \delta\mathbf{p}(t') = \delta\mathbf{q}(t'') = \delta\mathbf{p}(t'') = 0 \tag{1.8}$$

and the independence of $\delta\mathbf{q}$ and $\delta\mathbf{p}$ which V.P. is referred to as the modified Hamilton principle § yields the canonical (Hamilton) equations

$$dq^k/dt = \partial H/\partial p_k \tag{1.9}$$

$$dp_k/dt = -\partial H/\partial p^k \tag{1.10}$$

and hence

$$dH/dt = \partial H/\partial t \tag{1.11}$$

Of interest to this discussion of the quantum V.P. is what we would call the 'modified Hamilton homogeneous action principle' ‖ which yields equations (1.9), (1.10) and (1.11). For this V.P. one defines a linear functional $\mathscr{F}$

$$\mathscr{F}(\mathbf{q}, t, \mathbf{p}) = \int_{s'}^{s''} (p_k\,dq^k - H(\mathbf{q}, \mathbf{p}, t)\,dt) \tag{1.12}$$

† See, for example, Leech (1968) and Goldstein (1970), p. 58 and p. 30, respectively.
‡ For further discussion on the Gauteaux variation see, for example, Sagan (1969).
§ See, for example, Leech (1968) and Goldstein (1970), p. 58 and p. 225, respectively.
‖ Cf. Mercier (1963), pp. 166 and 190.

and requires that $\mathscr{F}$ have vanishing Gauteaux variation for independent variations $\delta\mathbf{q}$, $\delta\mathbf{p}$ and δt which vanish at end-points s' and s''.

Although variational methods have been extensively used in quantum mechanics,† the development of the quantum analogues of these three action principles was overlooked prior to the classic work of Schwinger (1951, 1953, 1970). Schwinger dealt with operator lagrangians, but he simplified the discussion by requiring that such variations as $\delta\mathbf{q}$, $\delta\dot{\mathbf{q}}$, $\delta\mathbf{p}$ and δt commute with all other operators. The major achievements of Schwinger (1953, 1970) was his derivation of the canonical commutation relations via the modified Hamilton homogeneous action principle. However, Kiang *et al.* (1969) and Lin *et al.* (1970) were able to show that for the lagrangian

$$\bar{L}(\mathbf{q}, \dot{\mathbf{q}}) = \tfrac{1}{2}\dot{q}^j g_{jk}(\mathbf{q})\dot{q}^k - V(\mathbf{q}) \tag{1.13}$$

the equations of motion deduced by Schwinger (1951),

$$\frac{d}{dt}\frac{\partial \bar{L}}{\partial \dot{q}^k} - \frac{\partial \bar{L}}{\partial q^k} = 0 \qquad \text{(Schwinger)} \tag{1.14}$$

(refinements involving left- and right-handed derivatives are irrelevant) were in general inconsistent with the Hamilton–Heisenberg equations,

$$i\hbar\frac{dq^k}{dt} = [q^k, \bar{H}], \qquad i\hbar\frac{dp_k}{dt} = [p_k, \bar{H}] \tag{1.15}$$

for $\bar{H}$ as given by Schwinger (1953, 1970)

$$\bar{H} = \tfrac{1}{2}\{p_k, \dot{q}^k\} - \bar{L} \qquad \text{(Schwinger)} \tag{1.16}$$

and p_k defined as $\partial\bar{L}/\partial\dot{q}^k$. Lin *et al.* (1970) showed that it was not, for example, sufficient to replace $\bar{H}$ by some other form, perhaps differing from $\bar{H}$ by a function of $\mathbf{q}$. However, Lin *et al.* (1970) were able to suggest an appropriate modification: they restricted their discussion to the case of zero curvature ($R = 0$) so that an algebraic transformation to 'euclidean coordinates' for which $g_{jk} = \delta_{jk}$ was possible, to find as a consistent modification

$$\frac{d}{dt}\frac{\partial \bar{L}}{\partial \dot{q}^k} - \frac{\partial \bar{L}}{\partial q^k} = Q_k \tag{1.17}$$

where the discrepancy term Q_k has two components

$$Q_k = \Delta_k + Z_{,k} \tag{1.18}$$

where we denote the partial derivatives with respect to q^k, by $,k$. One has

$$\Delta_k = \frac{1}{i\hbar}[\bar{L}, p_k] - \frac{1}{i\hbar}[\tfrac{1}{2}\{p_m, \dot{q}^m\}, p_k] - \frac{\partial \bar{L}}{\partial q^k} \tag{1.19}$$

from which one deduced directly that

$$\Delta_k = \tfrac{1}{4}\hbar^2 (g^{jl} g_{jm,l})_{,n} g^{mn}_{,k} \tag{1.20}$$

† See, for instance, Yourgrau & Mandelstam (1972).

whilst Z was determined by Lin *et al.* (1970) to be

$$Z = \tfrac{1}{4}\hbar^2 g^{jk}\Gamma^m_{jn}\Gamma^n_{km} \tag{1.21}$$

The significance of Z was that it gave the 'error' term in H, so that in the case considered Lin *et al.* (1970) found

$$\bar{H} = \tfrac{1}{2}\{p_k, \dot{q}^k\} - Z - \bar{L} \qquad (\text{case } R = 0) \tag{1.22}$$

Since the paper by Lin *et al.* (1970), a number of papers by Sugano and his co-workers (Sugano (1971), Kimura (1972) and Ohtani (1972)) have been directed towards the task of deducing the quantum-Euler–Lagrange from an action principle involving operator variations. However, because of the excessive restrictions imposed on the q-number variations q^k, their formulations are seriously defective, as we have shown elsewhere (Cohen & Shaharir, 1973). Another very *ad hoc* approach to the consistency issue was made by Kawai (1972, 1973), who added arbitrary terms to the lagrangian $\bar{L}$ so that the Euler–Lagrange equation was maintained in the form given by Schwinger.

In this paper we formulate a general q-number variational principle for the action integral (1.1) where the integrand is a lagrangian operator defined by

$$L(\mathbf{q}, \dot{q}, t) = \tfrac{1}{2}(\dot{q}^j - A^j(\mathbf{q}))g_{jk}(\mathbf{q})(\dot{q}^k - A^k(q)) - V(\mathbf{q}, t) \tag{1.23}$$

being a generalisation of $\bar{L}$.

In Section 2, the general concept of q-number variation is defined in terms of Gauteaux variation. It is shown that the trivial extension of the classical Gauteaux variations leads to restrictions on δq^k, a q-number variation in the commutative coordinate operators $q^k (k = 1, \ldots, N)$, such that the commutator δq^j with q^k is an operator independent of $\dot{\mathbf{q}}$,

$$[q^k, \delta q^j] = i\hbar\beta^{jk}(q, t) \tag{1.24}$$

Further properties of β^{jk} are derived in Lemma 2. An elementary identity for a twice differentiable vector field $\mathbf{v}$ is derived in Lemma 3, an important result which will be used in the later section, 3.

In Section 3 an admissible variational principle is formulated in which the vector operator $\delta\mathbf{q}$ satisfies equation (1.24) and the other properties derived in Section 2. The discussion utilises a lagrangian L, defined in equation (1.23), which describes the motion of a point particle influenced by a 'magnetic potential' in addition to a scalar potential in a N-dimensional Riemannian space of arbitrary curvature. It is assumed that p_k, the partial derivative $\partial L/\partial\dot{q}^k$ of operator L with respect to q^k, satisfies the commutation relation,

$$[q^j, p_k] = i\hbar\delta_k{}^j \tag{1.25}$$

$$[p_j, p_k] = 0 = [q^l, q^m] \tag{1.26}$$

To determine the Euler–Lagrange equation for the quadratic lagrangian L, the double commutator $[[\delta q^j, \dot{q}^k], \dot{q}^l]$ is needed, this double commutator being derived directly from our definition of the admissible Gauteaux variation and equations (1.25)–(1.26). However at no stage do we specify the commutator

$[\delta q^j, \dot{q}^k]$ (as was done by Sugano (1971), Kimura-Sugano (1972) and Ohtani *et al.* (1972), in view of the result shown elsewhere (Cohen & Shaharir (1973) that such a specification is excessively restrictive and leads to contradictions. The Euler–Lagrange equation deduced, is in the special cases considered by Lin *et al.* where $L = \bar{L}$ and $R = 0$, the same as equation (1.17).

In Section 4 the results obtained in Sections 2 and 3 are discussed.

2. *Preliminary*

Following the definition of the classical Gauteaux variation, we define δ-variation on an operator $O(\mathbf{q})$ which is a function of a set of commutative coordinate operators q^k $(k = 1, \ldots, N)$ by the limit

$$\delta O(\mathbf{q}; \delta\mathbf{q}) = \lim_{\epsilon \to 0} \frac{O(\mathbf{q} + \epsilon\, \delta\mathbf{q}) - O(\mathbf{q})}{\epsilon} \tag{2.1}$$

We will also assume the following 'derivative properties':

(a)
$$\delta O(\mathbf{q}; \delta\mathbf{q}) = \frac{1}{2}\left\{\frac{\partial O(\mathbf{q})}{\partial q^k}, \delta q^k\right\} \tag{2.2}$$

where $\{A, B\}$ denotes the anti-commutator, $AB + BA$, and the partial derivative $\partial O(\mathbf{q})/\partial q^k$ or $O_{,k}(\mathbf{q})$ is defined in the usual way.

$$O_{,k}(\mathbf{q}) = \frac{\partial O(\mathbf{q})}{\partial q^k} = \lim_{\boldsymbol{\sigma} \to 0} \frac{O(\mathbf{q} + \boldsymbol{\sigma}) - O(\mathbf{q})}{\|\boldsymbol{\sigma}\|} \tag{2.3}$$

in which the vector $\boldsymbol{\sigma}$ is a c-number whose component is non-zero at the kth position, and $\|\ \|$ is the euclidean norm.

(b)
$$\delta(AB)(\mathbf{q}; \delta\mathbf{q}) = \tfrac{1}{2}\{A(\mathbf{q}), \delta B(\mathbf{q}; \delta\mathbf{q})\} + \tfrac{1}{2}\{B(\mathbf{q}), \delta A(\mathbf{q}; \delta\mathbf{q})\} \tag{2.4}$$

where A and B are any operator functions of $\mathbf{q}$.

Consequently, there exists a class of admissible variation $\delta\mathbf{q}$, on the coordinate operator $\mathbf{q}$. Consider the particular operator given by $O(q) = q^3$, for which

$$\begin{aligned}\delta O(q; \delta q) &= \delta q q^2 + q^2\, \delta q + q\, \delta q q \\ &= \tfrac{1}{2}\{\delta q, 3q^2\} + \tfrac{1}{2}[[q, \delta q], q]\end{aligned}$$

where $[A, B]$ denotes the commutator $AB - BA$. In this case it is clear that equation (2.2) is valid if and only if the commutator of $\delta\mathbf{q}$ with $\mathbf{q}$ is a function of $\mathbf{q}$ and possibly t. More generally, it is possible to show (by induction) that the condition

$$[q^j, \delta q^k] = i\hbar\beta^{jk}(\mathbf{q}, t) \tag{2.5}$$

is necessary and sufficient for the validity of equation (2.2), for all 'analytic' operators $O(\mathbf{q})$. Further, by applying the definition of the δ-variation to the particular functional $[q^j, q^k]$, we can deduce the symmetric property of β^{jk}. The following result is trivial.

Lemma 1. Equations (2.1) and (2.2) imply equation (2.4) provided (if and only if) $\delta \mathbf{q}$ satisfies equation (2.5).

Equation (2.5) implies that $\delta \mathbf{q}$ is linear in some variables p_k ($k = 1, \ldots, N$), the momentum operator which is canonical to the coordinate $\mathbf{q}$. Thus we write

$$\delta q^j = \alpha^j(\mathbf{q}, t) + \tfrac{1}{2}\{\beta^{jk}(\mathbf{q}, t), p_k\} \tag{2.6}$$

where

$$[p_k, p_j] = 0, \qquad [q^j, p_k] = i\hbar\, \delta^j_k \tag{2.7}$$

The variation on the space of operators $F(\mathbf{q}, \dot{\mathbf{q}})$ which depend on a coordinate operator $\mathbf{q}$ and a velocity operator $\dot{\mathbf{q}}$ is defined in a similar manner. Thus by assuming equation (1.4), we have

$$\delta F\left(\mathbf{q}, \dot{\mathbf{q}}; \delta\mathbf{q}, \frac{d}{dt}\delta\mathbf{q}\right) = \lim_{\epsilon \to 0} \frac{F\left(\mathbf{q} + \epsilon\,\delta\mathbf{q}, \dot{\mathbf{q}} + \epsilon \frac{d}{dt}\delta\mathbf{q}\right) - F(\dot{\mathbf{q}}, \mathbf{q})}{\epsilon} \tag{2.8}$$

where $\delta \mathbf{q}$ is assumed to satisfy the commutation relation (2.5). However, since $\mathbf{q}$ and $\dot{\mathbf{q}}$ are non-commutative operators, further conditions on $\delta \mathbf{q}$ are expected, so that the definition (2.8) is meaningful. Thus we obtain the following lemma.

Lemma 2. Suppose $\dot{\mathbf{q}}$, the velocity operator, and $\mathbf{p}$, the momentum operator, are related by an equation

$$p_j = \tfrac{1}{2}\{\dot{q}^k - A^k(\mathbf{q}), g_{jk}(\mathbf{q})\}$$

where $\det(g_{jk}) \neq 0$, then operators α^j and β^{jk} defined by equations (2.6) and (2.8) satisfy the following equations:

(a) $$g^{jl}\beta^{km}_{,l} - \beta^{jl}g^{km}_{,l} + g^{kl}\beta^{jm}_{,l} - \beta^{kl}g^{jm}_{,l} + g^{lm}\beta^{jk}_{,l} - \beta^{lm}g^{jk}_{,l} = 0$$

(b) $$g^{kl}\alpha^j_{,l} - \beta^{kl}A^j_{,l} + g^{jl}\alpha^k_{,l} - \beta^{jl}A^k_{,l} + \beta^{jk}_{,l}A^l - g^{jk}_{,l}\alpha^l + \frac{\partial \beta^{jk}}{\partial t} = 0$$

Proof. The results follow from the uniqueness of $\delta([q^j, \dot{q}^k])$, and equating coefficients of p_k. Q.E.D.

The following result will also be used in Section 3.

Lemma 3. Let v^j be a component of a vector field in a riemannian space whose metric tensor is g_{jk}. Then provided v^j is twice differentiable, it satisfies the equation

$$g^{jk}_{,l}v^l_{,jk} = (g^{jk}\Gamma^m_{jn}\Gamma^n_{km})_{,l}v^l + 2g^{kl}\Gamma^m_{jn}\Gamma^n_{km}v^j_{;l} - 2g^{jm}\Gamma^l_{jk}v^k_{;ml}$$

where Γ^j_{kl} is the usual Christoffel symbol.

Proof. By definitions of the covariant derivative,

$$v^l_{,j} = v^l_{;j} - \Gamma^l_{jm}v^m$$

Similarly

$$v^l_{,jk} = v^l_{;jk} - \Gamma^l_{jm} v^m_{;k} - \Gamma^l_{km} v^m_{;j} + \Gamma^m_{jk} v^l_{;m} + (\Gamma^l_{jn}\Gamma^n_{km} - \Gamma^l_{mj,k}) v^m$$

Thus

$$g^{jk}_{,l} v^l_{,jk} = g^{jk}_{,l} v^l_{;jk} + 2g^{jk}\Gamma^l_{jm}\Gamma^m_{ln} v^n_{;k} + g^{jk}_{,l}(\Gamma^l_{jn}\Gamma^n_{km} - \Gamma^l_{mj,k}) v^m \quad \text{(L3.1)}$$

where use has been made of the relation

$$g^{jk}_{,l} = -g^{km}\Gamma^j_{ml} - g^{jm}\Gamma^k_{lm} \quad \text{(L3.2)}$$

By using the definition of the Riemann curvature tensor R^j_{klm},

$$R^j_{klm} = -\Gamma^j_{kl,m} + \Gamma^j_{km,l} - \Gamma^j_{mn}\Gamma^n_{kl} + \Gamma^j_{ln}\Gamma^n_{km} \quad \text{(L3.3)}$$

and (L3.2), we obtain

$$g^{jk}_{,l}(\Gamma^l_{jn}\Gamma^n_{km} - \Gamma^l_{mj,k}) = (g^{jk}\Gamma^l_{jn}\Gamma^n_{kl})_{,m} + g^{jk}_{,l} R^l_{jmk} \quad \text{(L3.4)}$$

By similar calculation, and use of the relation

$$v^j_{;kl} - v^j_{;lk} = R^j_{mlk} v^m \quad \text{(L3.5)}$$

we deduce

$$g^{jk}_{,l} v^l_{;jk} = -2g^{jk}\Gamma^m_{kn} v^n_{;jm} - g^{jk}\Gamma^n_{jl} R^l_{mkn} v^m \quad \text{(L3.6)}$$

Using the results in (L3.4) and (L3.6), together with the identity

$$R^j_{klm} + R^j_{lmk} + R^j_{mkl} = 0 \quad \text{(L3.7)}$$

we obtain the required result. Q.E.D.

3. *Formulation of a q-Number Variational Principle*

Consider a model of a dynamical system whose lagrangian operator, L, is defined by

$$L(\mathbf{q}, \dot{\mathbf{q}}, t) = \tfrac{1}{2}(\dot{q}^j - A^j(\mathbf{q}))g_{jk}(\mathbf{q})(\dot{q}^k - A^k(\mathbf{q})) - V(\mathbf{q}, t) \quad (3.1)$$

where $\mathbf{q}$ and $\dot{\mathbf{q}}$ ($\equiv d\mathbf{q}/dt$) are coordinate operators and velocity operators respectively. (All operators are assumed to be hermitian.) Classically the lagrangian L may be thought of as representing the motion of a point particle in an N dimensional riemannian space endowed by the metric tensor g_{jk}, in the presence of a magnetic potential $\mathbf{A}$ and an external potential $W = Lt(\hbar \to 0)V$.

The partial derivative $\partial L/\partial q^k$ ($k = 1, \ldots, N$) of L with respect to $\dot{q}^k$ will be assumed to form a set of variables p_k ($k = 1, \ldots, N$), the momentum operators, which are canonical to q^k ($k = 1, \ldots, N$), i.e.

$$\frac{\partial L}{\partial \dot{q}^k} = \tfrac{1}{2}\{g_{jk}, \dot{q}^j - A^j\} \equiv p_k \quad (3.2)$$

$$[q^j, p_k] = i\hbar\delta^j_k \quad (3.3)$$

$$[q^j, q^k] = 0 \tag{3.4}$$

$$[p_k, p_j] = 0 \tag{3.5}$$

We assume that there is an action integral (operator) $\mathscr{A}$ defined by

$$\mathscr{A}(\mathbf{q}, \dot{\mathbf{q}}) = \int_{t'}^{t''} L(\mathbf{q}, \dot{\mathbf{q}}, t)\, dt \tag{3.6}$$

which contains all the information of the dynamical system during the time interval t' to t''. In other words the variation $\delta(d', t' \mid d'', t'')$ of the 'transformation function' $(d', t' \mid d'', t'')$ (inner product between two Dirac states $(d', t' \mid$ and $\mid d'', t''))$ is $(i/\hbar)(d', t' \mid \delta \mathscr{A} \mid d'', t'')$. Following Schwinger (1953, 1970), we postulate that

$$\delta(d', t' \mid = -\frac{i}{\hbar}(d', t' \mid J(t') \tag{3.7}$$

$$\delta \mid d'', t'') = +\frac{i}{\hbar} J(t'') \mid d'', t'') \tag{3.8}$$

so that

$$\delta \mathscr{A} = J(t'') - J(t') \tag{3.9}$$

where J is a hermitian operator.

We define the variation $\delta \mathscr{A}$ in the operator $\mathscr{A}$ as an admissible Gauteaux variation of $\mathscr{A}$ given by

$$\delta \mathscr{A}\left(\mathbf{q}, \dot{\mathbf{q}}; \delta\mathbf{q}, \frac{d}{dt}\delta\mathbf{q}\right) = \lim_{\epsilon \to 0} \frac{\mathscr{A}\left(\mathbf{q} + \epsilon\, \delta\mathbf{q}, \dot{\mathbf{q}} + \epsilon \frac{d}{dt}\delta\mathbf{q}\right) - \mathscr{A}(\mathbf{q}, \dot{\mathbf{q}})}{\epsilon} \tag{3.10}$$

where we have implicitly assumed equation (1.4) and more importantly

$$\delta q^j = \alpha^j(\mathbf{q}, t) + \tfrac{1}{2}\beta(t)\{g^{jk}(\mathbf{q}), p_k\} \tag{3.11}$$

Physically, the admissible variation (3.11) is quite natural for it may be conceived as the total infinitesimal change in $\mathbf{q}$ generated by an infinitesimal spatial-time translation and rotational translation. However, our assumption in (3.11) is motivated by the results obtained in Section 2. (Note that δq^j in (3.11) satisfies (2.5) and Lemma 2.)

Now by definition (3.10),

$$\delta\mathscr{A}\left(\mathbf{q},\dot{\mathbf{q}};\delta\mathbf{q},\frac{d}{dt}\delta\mathbf{q}\right)=\int_{t'}^{t''}\frac{1}{2}\left(X^j(\mathbf{q},\dot{\mathbf{q}})g_{jk}(\mathbf{q})\frac{d}{dt}\delta q^k\right)dt$$
$$+\int_{t'}^{t''}\frac{1}{2}\left(\frac{d}{dt}\delta q^k g_{jk}(\mathbf{q})X^j(\mathbf{q},\dot{\mathbf{q}})\right)dt$$
$$+\int_{t'}^{t''}\left(X^j(\mathbf{q},\dot{\mathbf{q}})\,\delta g_{jk}(\mathbf{q};\delta\mathbf{q})X^k(\mathbf{q},\dot{\mathbf{q}})\right)dt$$
$$-\int_{t'}^{t''}\left(X^j(\mathbf{q},\dot{\mathbf{q}})g_{jk}(\mathbf{q})\,\delta A^k(\mathbf{q};\delta\mathbf{q})\right)dt$$
$$-\int_{t'}^{t''}\left(\delta A^k(\mathbf{q};\delta\mathbf{q})g_{jk}(\mathbf{q})X^j(\mathbf{q},\dot{\mathbf{q}})\right)dt$$
$$-\int_{t'}^{t''}\delta V(\mathbf{q};\delta\mathbf{q})\,dt \tag{3.12}$$

where

$$X^j(\mathbf{q},\dot{\mathbf{q}})=\dot{q}^j-A^j(\mathbf{q}) \tag{3.13}$$

By using equations (2.1), (2.2) and (2.3) equation (3.12) may be reduced to

$$\delta\mathscr{A}\left(\mathbf{q},\dot{\mathbf{q}};\delta\mathbf{q},\frac{d}{dt}\delta\mathbf{q}\right)=\int_{t'}^{t''}dt\left(\frac{1}{2}\left\{\frac{\partial L}{\partial\dot{q}^k},\frac{d}{dt}\delta q^k\right\}+\frac{1}{2}\left\{\frac{\partial L}{\partial q^k},\delta q^k\right\}\right)$$
$$+\int_{t'}^{t''}\tfrac{1}{4}(C+D-E)\,dt \tag{3.14}$$

where

$$C=\left[\frac{d}{dt}\delta q^j,\,[g_{jk},X^k]\right] \tag{3.15}$$

$$D=X^j g_{jk,l}[\delta q^l,X^k]+[X^k,\delta q^l]g_{jk,l}X^j \tag{3.16}$$

and

$$E=A^j_{,k}[\delta q^k,g_{jl}X^l]+[X^l g_{jl},\delta q^k]A^j_{,k} \tag{3.17}$$

Now using equations (3.2)-(3.5), (3.11) and (3.13) we deduce the following commutation relations:

(a)
$$[\delta q^j, X^k] = i\hbar g^{kl}\alpha^j_{,l} + \frac{i\hbar}{2}\{p_n, \theta^{jkn}\} \tag{3.18}$$

where

$$\theta^{jkn} = \beta(t)(g^{kl}g^{jn}_{,l} - g^{jl}g^{kn}_{,l}) \tag{3.19}$$

(b)
$$[X^l, [\delta q^j, X^k]] = \hbar^2 g^{lm}(g^{kn}\alpha^j_{,n})_{,m} + \frac{\hbar^2}{2}\{p_n, g^{lm}\theta^{jkn}_{,m} - g^{ln}_{,m}\theta^{jkm}\} \tag{3.20}$$

These results are used to simplify C, D and E defined earlier. Thus we deduce

$$\begin{aligned} C = {} & \hbar^2(g^{jk}g_{jl,k})_{,m}g^{mn}\alpha^l_{,n} - \hbar^2\beta(t)g^{ln}(g^{jk}g_{lj,k})_{,m}A^m_{,n} \\ & + \hbar^2\beta(t)g^{ln}_{,m}(g^{jk}g_{lj,k})_{,n}A^m + \frac{\hbar^2}{2}(g^{jk}g_{lj,k})_{,n}g^{ln}\frac{d\beta(t)}{dt} \\ & + \frac{\hbar^2}{2}\{p_n, (g^{jk}g_{lj,k})_{,m}(\theta^{lmn} + \beta(t)g^{lm}_{,s}g^{ns})\} \end{aligned} \tag{3.21}$$

where use has also been made of the relation

$$\frac{dO(\mathbf{q}, t)}{dt} = \frac{1}{2}\left\{\frac{\partial O(\mathbf{q}, t)}{\partial q^k}, \dot{q}^k\right\} + \frac{\partial O(\mathbf{q}, t)}{\partial t} \tag{3.22}$$

Similarly, after some simplification, we obtain

$$\begin{aligned} D = {} & -\hbar^2 g^{jk}\alpha^l_{,jk} + \hbar^2(g^{lm}g_{jm,l})_{,k}g^{jn}\alpha^k_{,n} \\ & + \frac{\hbar^2}{2}\{p_n, g_{jm,k}(g^{lm}\theta^{kjn}_{,l} - g^{mn}_{,l}\theta^{kjl}) + g_{mj,kl}(g^{lm}\theta^{kjn} - g^{nm}\theta^{kjl})\} \end{aligned} \tag{3.23}$$

and

$$E = -\hbar^2\beta(t)g^{lm}_{,k}A^k_{,lm} + \hbar^2\beta(t)g^{lm}(g^{jk}g_{jn,k})_{,m}A^n_{,l} \tag{3.24}$$

Thus

$$\begin{aligned} C + D - E = {} & \hbar^2(g^{jk}g_{jm,k})_{,l}\Big(g^{ln}\alpha^m_{,n} - \beta(t)g^{ln}A^m_{,n} + g^{mn}\alpha^l_{,n} - \beta(t)g^{mn}A^l_{,n} \\ & + \beta(t)g^{lm}_{,n}A^n + g^{lm}\frac{d\beta(t)}{dt}\Big) + \frac{\hbar^2}{2}\{\{p_n, \beta(t)g^{nm}\}, g^{jk}_{,m}(g^{ls}g_{sj,l})_{,k}\} \\ & - \hbar^2(\alpha^k_{,ln} - \beta(t)A^k_{,ln})g^{ln}_{,k} + \frac{\hbar^2}{2}\{P_n, F^n\} \end{aligned} \tag{3.25}$$

where

$$\begin{aligned} F^n = {} & g_{mj,k}(g^{lm}\theta^{kjn}_{,l} - g^{mn}_{,l}\theta^{kjl}) + g_{mj,kl}(g^{lm}\theta^{kjn} - g^{mn}\theta^{kjl}) \\ & + (g^{jk}g_{mj,k})_{,l}\theta^{mln} \end{aligned} \tag{3.26}$$

But by Lemma 2 (Section 2), we have a relation

$$g^{jl}v^k_{,l} + g^{kl}v^j_{,l} - g^{jk}_{,l}v^l + g^{jk}\frac{d\beta(t)}{dt} = 0 \tag{3.27}$$

where

$$v^k = \alpha^k - \beta(t)A^k \tag{3.28}$$

Lemma 3 (Section 2) becomes

$$g^{jn}_{,k}v^k_{,lm} = \tfrac{1}{2}\{(g^{jk}\Gamma^m_{jn}\Gamma^n_{km})_{,l}, v^l\} - g^{jk}\Gamma^m_{jn}\Gamma^n_{km}\frac{d\beta}{dt} \tag{3.29}$$

where use has been made of the equivalent form of (3.27), namely

$$g^{jl}v^k_{;l} + g^{kl}v^j_{;l} + g^{jk}\frac{d\beta}{dt} = 0 \tag{3.30}$$

Further, using (3.2), (3.11) and (3.22) equation (3.29) becomes

$$g^{jn}_{,k}v^k_{,lm} = \tfrac{1}{2}\{(g^{jk}\Gamma^m_{jn}\Gamma^n_{km})_{,l}, \delta q^l\} - \frac{d}{dt}(\beta(t)g^{jk}\Gamma^m_{jn}\Gamma^n_{km}) \tag{3.31}$$

Using equations (2.27), (2.28) and (3.31), equation (3.25) now may be written as

$$C + D - E = \frac{\hbar^2}{2}\{(g^{jk}g_{jm,k})_{,l}g^{lm}_{,n} - (g^{jk}\Gamma^m_{jn}\Gamma^n_{km})_{,n}, \delta q^n\}$$

$$+\hbar^2\frac{d}{dt}(\beta(t)g^{jk}\Gamma^m_{jn}\Gamma^n_{km}) + \frac{\hbar^2}{2}\{P_m, F^m\} \tag{3.32}$$

However in the appendix it is shown that F^n is identical to zero. Thus equation (3.14) now becomes

$$\delta\mathscr{A}\left(\mathbf{q}, \dot{\mathbf{q}}; \delta\mathbf{q}, \frac{d}{dt}\delta\mathbf{q}\right) = \int_{t'}^{t''} dt\left(\frac{1}{2}\frac{d}{dt}\left(\left\{\frac{\partial L}{\partial\dot{q}^k}, \delta q^k\right\} + \frac{\hbar^2}{2}\beta(t)g^{jk}\Gamma^m_{jn}\Gamma^n_{km}\right)\right)$$

$$-\int_{t'}^{t''} dt\left(\left\{\frac{d}{dt}\frac{\partial L}{\partial\dot{q}^k} - \frac{\partial L}{\partial q^k} - Q_k, \delta q^k\right\}\right) \tag{3.33}$$

where

$$Q_k = \frac{\hbar^2}{4}(g^{jl}g_{jm,l})_{,n}g^{mn}_{,k} - \frac{\hbar^2}{4}(g^{jk}\Gamma^m_{jn}\Gamma^n_{km})_{,k} \tag{3.34}$$

Schwinger's principle (3.9) allows us to identify the generator

$$J = \tfrac{1}{2}\left\{\frac{\partial L}{\partial\dot{q}^k}, \delta q^k\right\} + \frac{\hbar^2}{4}\beta(t)g^{jk}\Gamma^m_{jn}\Gamma^n_{km} \tag{3.35}$$

and the quantal Euler–Lagrange equation

$$L_k = \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^k} - \frac{\partial L}{\partial q^k} - Q_k = 0 \tag{3.36}$$

4. *Discussion*

We have derived the quantal Euler–Lagrange equation $L_k = 0$ via a variational principle in which the variation $\delta\mathbf{q}$ in the coordinate operator $\mathbf{q}$ is given by

$$\delta q^k = \alpha^k(\mathbf{q}, t) + \frac{1}{2}\left\{\frac{\partial L}{\partial \dot{q}^j}, \beta(t) g^{jk}\right\} \tag{4.1}$$

where q^k and $\partial L/\partial \dot{q}^k \equiv p_k$ are canonical conjugate variables. We consider this variation, although not quite the most general, in view of the incredible clumsiness entailed by the most general form of admissible variation

$$\delta q^k = \alpha^k(\mathbf{q}, t) + \frac{1}{2}\left\{\beta^{jk}(t, \mathbf{q}), \frac{\partial L}{\partial \dot{q}^j}\right\} \tag{4.2}$$

for some symmetric tensor β^{jk} which satisfies Lemma 2. A detailed calculation given elsewhere† shows that in the case where $\mathbf{A} = 0$, β^{jk} must satisfy the constraint

$$F^s + g^{sr}\beta^{jk}_{,r}(g^{lm}g_{mj,l})_{,k} + g^{rs}(\beta^{jm}\Gamma^l_{jm}\Gamma^k_{lm} + \beta^{jk}_{,l}\Gamma^l_{jk})_{,r}$$
$$= g^{jk}_{,n}(g^{lm}g_{lj,m})_{,k}\beta^{ns} - \beta^{ns}(g^{jk}\Gamma^l_{jm}\Gamma^m_{kl})_{,n} \tag{4.3}$$

where F^s is the same functional form as (3.26), but θ^{jk} takes the form

$$\theta^{jkl} = \beta^{km}g^{jl}_{,m} - g^{jm}\beta^{kl}_{,m} \tag{4.4}$$

In the above derivation (Section 3), we have proceeded from the equation

$$\{L_k, \delta q^k\} = 0 \tag{4.5}$$

to deduce

$$L_k = 0 \tag{4.6}$$

Implicit in this step is the lemma proved in a lengthy calculation by Shaharir (1974b):

$$[L_k, \delta q^k] = 0 \tag{4.7}$$

Consequently, it follows from (4.5) that

$$L_k\,\delta q^k = 0 \tag{4.8}$$

so that, provided δq^k is non-singular, one may properly deduce equation (4.6) (the Euler–Lagrange equation).

† Shaharir (1974b).

Even though we have succeeded in formulating a q-number variational principle precisely analogous to the Hamilton variational principle, we wonder whether such a formulation is the most appropriate basis for quantum mechanics. Our personal preference is to dispense with the formal integrals, and to assert in lieu of (3.9) the principle that Gauteaux variation δL is a total derivative, i.e.

$$\delta L = \frac{d}{dt} J \tag{4.9}$$

This starting point leaves the critical parts of the above calculations unchanged. In fact, a close examination of the integral expressions raises various points which, though no doubt resolvable, are a cause for concern. For example, if one naïvely presumed that the q^k were in the Schroedinger picture, it would follow that the integrand had no time dependence at all, and the integration, especially the integration by parts, would be a mere formal device.

One unexpected feature of our calculation is that, unlike Schwinger, we find that the hermitian operator J in equation (4.9) is not in general simply related to that infinitesimal transformational generator G for which

$$[\mathrm{q}^k, G] = i\hbar\, \delta \mathrm{q}^k$$

Consequently, in quantum mechanics on a riemannian manifold, there is not a one-to-one correspondence between symmetry transformations and conserved currents, i.e. Noether's theorem cannot be stated 'strongly'. This conclusion compliments the work of Rosen (1971, 1972) on Noether's theorem in classical field theory.

We should mention that the classical V.P. has a very elegant reformulation in the language of differential forms whereby the variation is translated as the Cartan (exterior) differential mapping on a symplectic (contact) manifold.† However, the extension to quantum mechanics of this coordinate free notation would require the development of calculus of exterior differential forms over a non-abelian ring, as a 'wedge product' such as $dq^j \wedge dq_k$ would not be antisymmetric.

In this paper, we had only discussed the variational principle as applied to the action integral (3.6). This may be referred as the 'Hamilton–Schwinger q-number Variational Principle'. Elsewhere, one of us (Shaharir, 1974a) has presented the action principle which is termed the 'Modified Hamilton–Schwinger (Homogeneous) Variational Principle'. It was found possible to derive the Hamilton–Heisenberg equations (1.15) via a q-number variational principle which is consistent with the one developed here. In addition it was shown that the derivation of the canonical commutation relation C.C.R. via the method of the Schwinger action principle (1953, 1970) is possible only if $g_{jk} = \delta_{jk}$, i.e. for those lagrangians for which Schwinger's c-number variational principles can be consistently formulated.

† See, for instance, Hermann (1965).

Appendix

We wish to show that the functional F^n defined by equation (3.26), Section 3, is identical to zero. It is sufficient to consider

$$\bar{F}^n = g_{mj,k}(g^{ml}\bar{\theta}^{kjn}_{,l} - g^{mn}_{,l}\bar{\theta}^{kjl}) + g_{mj,kl}(g^{lm}\bar{\theta}^{kjn} - g^{mn}\bar{\theta}^{kjl}) + (g^{jk}g_{mj,k})_{,l}\bar{\theta}^{mln} \qquad \text{(A.1)}$$

where

$$\bar{\theta}^{kln} = g^{mn}_{,k}g^{kl} - g^{ln}_{,k}g^{km} \qquad \text{(A.2)}$$

The first two terms of (A.1) are equivalent to

$$(g^{nm}(g_{lj,k}\bar{\theta}^{kj}_m - g_{mj,k}\bar{\theta}^{kj}_l))_{,s}g^{sl} + g_{sj,k}g^{sn}g^{lm}\bar{\theta}^{kj}_{m,l}$$

where we have defined $\bar{\theta}^{kj}_m = g_{lm}\bar{\theta}^{kjl}$. But by definition of $\bar{\theta}^{kj}_m$ and using the usual expression of $g_{jk,l}$ and $g^{jk}_{,l}$ in terms of the Christoffel symbols, Γ^{j}_{ul}, it can be shown that

$$g_{lj,k}\bar{\theta}^{kj}_m - g_{mj,k}\bar{\theta}^{kj}_l = 0.$$

Thus $\bar{F}^n$ now becomes

$$\bar{F}^n = (g_{sj,k}g^{lm}\bar{\theta}^{kj}_{m,l} + (g^{jk}g_{mj,k})_{,l}\bar{\theta}^{ml}_s)g^{sn} \qquad \text{(A.3)}$$

Again by definition of $\bar{\theta}^{kj}_m$, we have

$$g_{sj,k}g^{lm}\bar{\theta}^{kj}_{m,l} = (g_{sj,k} - g_{sk,j})g^{lm}(g_{mr}g^{kr}_{,n}g^{jn})_{,l} = (g_{sj,k} - g_{sk,j})(g^{jn}g^{kl}_{,nl} + g^{lm}g^{kr}_{,n}g^{jn}g_{mr,l}) \qquad \text{(A.4)}$$

Similarly,

$$(g^{jk}g_{jm,k})_{,l}\bar{\theta}^{ml}_s = (g^{jk}g_{jm,l})(g^{ln}g_{ns,r}g^{mr} - g^{mn}g_{ns,r}g^{lr}) \qquad \text{(A.5)}$$

where use has also been made of the identity

$$g^{jk}_{,l} = -g^{jr}g^{ks}g_{rs,l} \qquad \text{(A.6)}$$

Simplifying (A.5) further, and applying (A.6) we arrive at

$$(g^{jk}g_{mj,k})_{,l}\bar{\theta}^{ml}_s = g^{ln}g_{ns,r}(-g^{kr}_{,kl} - g^{jk}g_{mj,k}g^{mr}_{,l} + g^{lr}g_{ns,r}(g^{kn}_{,kl} + g^{jk}g_{mj,k}g^{mn}_{,l}) \qquad \text{(A.7)}$$

which is the 'inverse' of (A.4).

The result follows from (A.3), (A.4) and (A.7). Q.E.D.

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