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On Consistency between Lagrange and Hamilton Formalisms in Quantum Mechanics

——*Case of Non-Relativistic Velocity-Dependent Potential*——

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Consistency between the Lagrangean and the Hamiltonian formalisms in the quantum mechanics is investigated for the type of Lagrangean $L=\frac{1}{2}\dot{q}_i g_{ij}(q)\dot{q}_j-v(q)$ as an extension of a previous paper. The variations δq_i and $\delta\dot{q}_i$ should be considered as q-numbers. When the Lagrangean can be transformed into the standard form $L=\frac{1}{2}\dot{Q}_\alpha{}^2-V(Q)$, the commutation relations of δq_i and $\delta\dot{q}_i$ with q_j and $\dot{q}_j$ are found with the help of the Q-coordinate system. It is shown that using the commutation relations, the variation principle leads to the same equation of motion as the canonical equation of motion which is obtained in the previous paper.

§ 1. Introduction

For velocity-dependent potentials, the ordinary procedure obtaining a Hamiltonian and an equation of motion does not lead to a consistent result for the Lagrangean and the Hamiltonian formalism, though both formalisms have no contradiction each other in the classical mechanics. This fact is due to the ambiguity of an ordering of operators. In previous works,[1),2)] the type of Lagrangean $L=\frac{1}{2}\dot{q}_i g_{ij}\dot{q}_j-v(q)$ was investigated[*)] where $g_{ij}=g_{ji}$ is a function of $q_i(i=1\sim n)$. It was shown that in the quantum mechanics, the correct Hamiltonian should be[**)] $H=\frac{1}{2}\{p_i, \dot{q}_i\}-L-Z(q)$ with Z expressed in terms of g_{ij} and its derivative, and this H satisfied the canonical equation of motion. The equation of motion for q_i, however, could not be derived from the ordinary variation principle due to the fact that $\delta\dot{q}_i$ was a q-number. The proposed formalism was examined for some examples (the free Lagrangean for the polar coordinate system, etc.). If there exists the canonical transformation from q_i to $Q_\alpha(\alpha=1\sim n)$ for which the Lagrangean has standard form $L=\frac{1}{2}\dot{Q}_\alpha{}^2-V(Q)$, the consistent equation of motion is derived from the equation for Q_α. It was indicated in I that the Euler-Lagrange equation should be modified and that the ordinary variational method was not valid.

In this paper, it is, however, proved that if δq_i and $\delta\dot{q}_i$ are appropriately regarded as q-numbers, the variation principle yields the consistent equation of

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*) The summation convention is assumed for dummy indices.

**) In this paper, the curly and the square brackets denote the anti-commutator and the commutator, respectively.

motion. In § 2, a brief review of I is presented in a slightly modified way. In § 3, it is shown that the ordinary definition of canonical momentum and its commutation relation with q_i are not independent assumptions in this case as well as in the standard Lagrangean, provided that the canonical equation of motion is accepted. In § 4, the commutation relations of δq_i and $\delta\dot{q}_i$ with q_j and $\dot{q}_j$ are given and with the aid of these commutators, the Euler-Lagrange equation is derived by means of the variational method. Section 5 is devoted to discussion of the result. Complicated calculations in the text are given in the Appendices.

§ 2. Summary of the previous work

Let us first summarize essential points in the previous work in a slightly different way for the convenience of the following argument. The initial Lagrangean is given by

$$L=\tfrac{1}{2}\dot{q}_i g_{ij}(q)\dot{q}_j-v(q), \qquad (i=1\sim n) \tag{2·1}$$

where q_i and $\dot{q}_i$ stand for a generalized coordinate operator and its time derivative, respectively. $g_{ij}(q)$ is symmetric with respect to i and j for the Lagrangean to be hermitian and g_{ij} and V are functions of only $q_i (i=1\sim n)$.

The canonical momentum conjugate to q_i is defined by

$$p_i=\frac{\partial L}{\partial \dot{q}_i}=\frac{1}{2}\{\dot{q}_j, g_{ij}(q)\}, \tag{2·2}$$

and is assumed to satisfy the canonical commutation relation

$$[p_i, q_j]=-i\delta_{ij}, \tag{2·3}$$

and all other commutators vanish. From (2·2) and (2·3), it follows that

$$[\dot{q}_i, q_j]=-if_{ij}(q), \tag{2·4}$$

if $[\dot{q}_i, q_j]$ is a function of q_k only, where f_{ij} is also symmetric in i and j and is related to g_{ij} with

$$f_{ij}(q)g_{jk}(q)=g_{ij}(q)f_{jk}(q)=\delta_{ik}, \tag{2·5}$$

provided that det $(g_{ij})\neq 0$. (2·2) and (2·3) were the fundamental assumptions in I. The assumptions are, however, not independent ones if the canonical equation of motion is accepted and the commutators $[p_i, q_j]$ and $[\dot{q}_i, q_j]$ are functions of q_k only. The proof will be given in § 3.

Owing to (2·4) in which $f_{ij}(q)$ is not a c-number, $\delta\dot{q}_i$ is in general a q-number. This fact gives rise to the difficulty that the Lagrange formalism is not consistent with the Hamilton one. In order to avoid the trouble, the transformation of variables is introduced by which the Lagrangean is brought into the standard form

$$L=\tfrac{1}{2}\dot{Q}_\alpha^2-V(Q), \qquad (\alpha=1\sim n) \tag{2·6}$$

with*)

$$Q_\alpha = Q_\alpha(q), \qquad \dot{Q}_\alpha = \frac{1}{2}\left\{\dot{q}_i, \frac{\partial Q_\alpha}{\partial q_i}\right\}, \tag{2·7}$$

if the following condition is satisfied:

$$\frac{\partial q_i}{\partial Q_\alpha}\frac{\partial q_j}{\partial Q_\beta} g_{ij} = \delta_{\alpha\beta}\,. \tag{2·8}$$

Then the commutation relation is transformed to

$$[P_\alpha, Q_\beta] = [\dot{Q}_\alpha, Q_\beta] = -i\delta_{\alpha\beta} \tag{2·9}$$

and all others vanish.

The consistency between $[p_i, q_j]$ (or $[\dot{q}_i, q_j]$) and $[P_\alpha, Q_\beta]$ is guaranteed by (2·7) and (2·8). The transformation (2·7) can be expressed also in terms of P_α, Q_α, p_i and q_i:

$$Q_\alpha = Q_\alpha(q), \qquad P_\alpha = \frac{1}{2}\left\{p_i, \frac{\partial q_i}{\partial Q_\alpha}\right\} \tag{2·10}$$

or

$$q_i = q_i(Q), \qquad p_i = \frac{1}{2}\left\{P_\alpha, \frac{\partial Q_\alpha}{\partial q_i}\right\}. \tag{2·11}$$

Since, for the standard Lagrangean (2·6), the Lagrange formalism is consistent with the Hamilton one, the correct Hamiltonian is defined by

$$H(P, Q) = P_\alpha \dot{Q}_\alpha - L(Q, \dot{Q}), \tag{2·12}$$

which is different from

$$K(p, q) \equiv \tfrac{1}{2}\{p_i, \dot{q}_i\} - L(q, \dot{q}). \tag{2·13}$$

H and K are related by

$$H(p, q) = K(p, q) - Z(q), \tag{2·14}$$

where

$$\begin{aligned} Z(q) &= -\dot{Q}_\alpha{}^2 + \tfrac{1}{2}\{p_i, \dot{q}_i\} \\ &= \frac{1}{4}\left[p_i, \frac{\partial q_j}{\partial Q_\alpha}\right]\left[p_j, \frac{\partial q_i}{\partial Q_\alpha}\right]. \end{aligned} \tag{2·15}$$

With the help of (2·8), Z can be expressed in terms of f_{ij} and g_{ij}

$$Z = -\frac{1}{16} f_{ij} f_{kl} f_{mn} \frac{\partial g_{ij}}{\partial q_m}\frac{\partial g_{kl}}{\partial q_n} - \frac{1}{4}\frac{\partial}{\partial q_i}\left(f_{ij} f_{kl}\frac{\partial g_{kl}}{\partial q_j}\right) - \frac{1}{4}\frac{\partial^2 f_{ij}}{\partial q_i \partial q_j} \tag{2·16a}$$

or

$$= -\frac{1}{16} f_{ij}\frac{\partial f_{kl}}{\partial q_i}\frac{\partial g_{kl}}{\partial q_j} + \frac{1}{8} f_{ij}\frac{\partial f_{kl}}{\partial q_i}\frac{\partial g_{jl}}{\partial q_k}\,. \tag{2·16b}$$

*) $\partial Q_\alpha/\partial q_i$ and $\partial q_i/\partial Q_\alpha$ are understood to be $i[p_i, Q_\alpha]$ and $i[P_\alpha, q_i]$, respectively.

The first expression (2·16a) was obtained in I, the second one (2·16b) is derived in Appendix B. It is noticed that Z does not depend on $\dot{q}_i$ or p_i. As the two forms of Z are not identical, (2·16a) and (2·16b) impose a condition for f_{ij} or g_{ij} to satisfy (2·8). In other words, for the only f_{ij} or g_{ij} for which (2·16a) and (2·16b) coincide,*) there exists the transformation (2·7) or (2·10) leading to the standard Lagrangean (2·6).

From the canonical equations of motion

$$\dot{Q}_\alpha = i[H, Q_\alpha], \qquad \dot{P}_\alpha = i[H, P_\alpha] \tag{2·17}$$

or from the Euler-Lagrange equation

$$\frac{d}{dt}\frac{\partial L(Q,\dot{Q})}{\partial \dot{Q}_\alpha} - \frac{\partial L(Q,\dot{Q})}{\partial Q_\alpha} = 0\,, \tag{2·18}$$

transforming back P_α and Q_α into p_i and q_i (or $\dot{q}_i$ and q_i), one can obtain

$$\dot{q}_i = i[H, q_i], \qquad \dot{p}_i = i[H, p_i] \tag{2·19}$$

and

$$\frac{d}{dt}\frac{\partial L(q,\dot{q})}{\partial \dot{q}_i} - \frac{\partial L(q,\dot{q})}{\partial q_i} = \frac{\partial Z}{\partial q_i} + \frac{1}{4}\frac{\partial f_{jk}}{\partial q_i}\frac{\partial}{\partial q_k}\left(f_{lm}\frac{\partial g_{jl}}{\partial q_m}\right). \tag{2·20}$$

Hence, the Hamiltonian H is the time generator of the (p, q) system and its eigenvalue gives an energy of the system. The extra terms in (2·20) are due to the fact that δq_i and $\delta \dot{q}_i$ are q-numbers (see § 4). The Euler-Lagrange equation looks in appearance as if the system is non-conservative, however, (2·18) indicates that the system is conservative if (2·8) is satisfied.

§ 3. Definition of canonical momentum and commutation relation

In this section, it is proved that the definition of canonical momentum (2·2) and the commutation relation (2·3) are not independent assumptions for the Lagrangean (2·1), but one of them requires another one under the following conditions:

(i) the canonical equation of motion (2·19) is valid,

(ii) the Hamiltonian is defined by

$$H = \tfrac{1}{2}\{p_i, \dot{q}_i\} - L - A\,, \tag{3·1}$$

where A is an arbitrary function of q_i,

(iii) the commutators $[p_i, q_j]$ and $[\dot{q}_i, q_j]$ are independent of $\dot{q}_k$:

*) In fact, for examples for which explicit forms of the transformation are known, (2·16a) and (2·16b) yield the same Z. As the special example, putting $g_{ij} = g\delta_{ij}$, $f = g^{-1}$, one obtains the relation from (2·16)

$$(n^2+n-2)\left(\frac{\partial f}{\partial q_i}\right)^2 = 4(n-1)\frac{\partial^2 f}{\partial q_i^2} f\,.$$

This is not satisfied with an arbitrary f except the case $n=1$.

$$[p_i, q_j] = \xi_{ij}(q), \qquad [\dot{q}_i, q_j] = \eta_{ij}(q). \tag{3·2}$$

From the conditions (i), (ii) and (iii) it follows that

$$\dot{q}_i = i[H, q_i] = \frac{i}{2}\{\xi_{ji}, \dot{q}_j\} + \frac{i}{2}\{p_j, \eta_{ji}\} - i[L, q_i]. \tag{3·3}$$

Here one has

$$[L, q_i] = \frac{1}{2}\eta_{ji} g_{jk} \dot{q}_k + \frac{1}{2}\dot{q}_j g_{jk} \eta_{ki} = \frac{1}{2}\left\{\eta_{ji}, \frac{\partial L}{\partial \dot{q}_j}\right\}, \tag{3·4}$$

where

$$\frac{\partial L}{\partial \dot{q}_i} = \frac{1}{2}\{g_{ij}, \dot{q}_j\}. \tag{3·5}$$

Substituting (3·4) into (3·3), one finds

$$\{\dot{q}_j, \xi_{ji} + i\delta_{ij}\} + \left\{p_j - \frac{\partial L}{\partial \dot{q}_j}, \eta_{ji}\right\} = 0. \tag{3·6}$$

Thus, due to (3·6), if $p_i = \partial L/\partial \dot{q}_i$, then $\xi_{ij} = -i\delta_{ij}$ and *vice versa.*

A modification of the commutation relation, therefore, cannot remove away the difficulty mentioned in § 1, if the definition of canonical momentum (2·3) and Hamiltonian (3·1) are employed.

§ 4. Euler-Lagrange equation and variation principle in q-system

If the transformation (2·10) or (2·11) exists in the Q-coordinate system, variations δQ_α and $\delta \dot{Q}_\alpha$ can be regarded as c-numbers. But δq_i and $\delta \dot{q}_i$ cannot be taken as c-numbers. Since one has

$$\delta q_i = \frac{\partial q_i}{\partial Q_\alpha}\delta Q_\alpha, \tag{4·1}$$

$$\delta \dot{q}_i = \frac{1}{2}\left\{\delta \dot{Q}_\alpha, \frac{\partial q_i}{\partial Q_\alpha}\right\} + \frac{1}{2}\left\{\dot{Q}_\alpha, \frac{\partial^2 q_i}{\partial Q_\alpha \partial Q_\beta}\delta Q_\beta\right\}, \tag{4·2}$$

δq_i and $\delta \dot{q}_i$ do not commute with $\dot{q}_i$ when δQ_α and $\delta \dot{Q}_\alpha$ are c-numbers. Differentiating (4·1) with respect to time, one easily sees*)

$$\frac{d}{dt}\delta q_i = \delta \dot{q}_i. \tag{4·3}$$

This fact (4·3) makes the variational principle applicable to this case. In fact, if one treats δq_i and $\delta \dot{q}_i$ as q-numbers in the variational method, it is snown that

*) In I, (4·3) did not hold as δq_i was assumed to be a c-number, although this assumption was not used in the calculation there. The consequence of I, therefore, does not need to be changed. Suppose δQ_α and $\delta \dot{Q}_\alpha$ to be c-numbers, then one must put both δq_i and $\delta \dot{q}_i$ into q-numbers.

the consistent equation of motion (2·20) can be derived from

$$\delta\int_{t_1}^{t_2} L(q,\dot q)\,dt=0\,. \tag{4·4}$$

Before doing this, one has to obtain the commutation relations $[q_i, \delta\dot q_j]$, $[\delta q_i, \dot q_j]$ and $[\dot q_i, \delta\dot q_j]$. However, there is no general criterion to settle these commutators only in the q-system. Since δQ_α and $\delta\dot Q_\alpha$ are c-numbers, one can obtain these commutators with the help of (4·1) and (4·2). The derivation is shown in Appendix B and the result is

$$[q_i, \delta q_j]=0\,, \tag{4·5}$$

$$[\dot q_i, \delta q_j]=-[q_i, \delta\dot q_j]=\frac{i}{2}f_{ik}f_{jl}G_{klm}\delta q_m\,, \tag{4·6}$$

$$[\dot q_i, \delta\dot q_j]=\frac{i}{4}\delta\{f_{ik}f_{jl}G_{klm}, \dot q_m\}+\frac{i}{8}\{(f_{ik}f_{jl}+f_{jk}f_{il})f_{mn}G_{mkr}G_{nls}\delta q_s, \dot q_r\} \tag{4·7}$$

with

$$G_{klm}=G_{mlk}=\frac{\partial g_{lm}}{\partial q_k}-\frac{\partial g_{km}}{\partial q_l}+\frac{\partial g_{kl}}{\partial q_m}\,. \tag{4·8}$$

The commutator (4·6) is in accord with (2·4) as is seen by taking variation of (2·4). The i-j anti-symmetric part of (4·7) is also consistent with the commutator

$$[\dot q_i, \dot q_j]=\frac{i}{2}\{f_{ik}f_{jl}G_{[kl]m}, \dot q_m\}$$

which is obtained from (2·3) and (2·2). Here $G_{[kl]m}$ denotes the k-l anti-symmetric part of G_{klm}; $G_{[kl]m}=\partial g_{lm}/\partial q_k-\partial g_{km}/\partial q_l$. In (4·6) and (4·7) commutators of δq_i and $\delta\dot q_i$ are coupled with other component of variation δq_k $(k\neq i)$.

With these preparations, one can now proceed to the variational method. The variation of the Lagrangean (2·1) is

$$\delta L(q,\dot q)=\frac{1}{2}\,(\delta\dot q_i g_{ij}\dot q_j+\dot q_i g_{ij}\delta\dot q_j)+\frac{1}{2}\dot q_i\frac{\partial g_{ij}}{\partial q_k}\delta q_k\dot q_j-\frac{\partial v}{\partial q_k}\delta q_k\,. \tag{4·9}$$

By using (4·5) ~ (4·7), all δq_i and $\delta\dot q_i$ can be shifted to the right. After a lengthy calculation, one finds

$$\delta L(q,\dot q)=\frac{\partial L}{\partial\dot q_a}\delta\dot q_a+\frac{\partial L}{\partial q_a}\delta q_a+\frac{i}{4}\frac{d}{dt}(g_{ij}\delta f_{ij})+\{\dot q_i, R_{ia}\delta q_a\}+S_a\delta q_a\,, \tag{4·10}$$

where

$$R_{ia}\equiv\frac{-i}{4}f_{kl}f_{mn}\frac{\partial g_{ik}}{\partial q_n}G_{[lm]a}-\frac{i}{8}\frac{\partial f_{kl}}{\partial q_a}\frac{\partial g_{kl}}{\partial q_i}-\frac{i}{8}f_{kl}f_{mn}G_{ikm}G_{aln}\,, \tag{4·11}$$

$$S_a = -\frac{1}{16}\frac{\partial}{\partial q_a}\left(f_{kl}\frac{\partial f_{ij}}{\partial q_k}\frac{\partial g_{ij}}{\partial q_l}\right)+\frac{1}{8}\frac{\partial}{\partial q_a}\left(f_{ij}\frac{\partial f_{kl}}{\partial q_i}\frac{\partial g_{jl}}{\partial q_k}\right)+\frac{1}{4}\frac{\partial f_{ik}}{\partial q_a}\frac{\partial}{\partial q_k}\left(f_{jl}\frac{\partial g_{ij}}{\partial q_l}\right)$$

$$=\frac{\partial Z}{\partial q_a}+\frac{1}{4}\frac{\partial f_{ik}}{\partial q_a}\frac{\partial}{\partial q_k}\left(f_{jl}\frac{\partial g_{ij}}{\partial q_l}\right). \tag{4·12}$$

From the relation

$$f_{ij}\frac{\partial g_{ij}}{\partial q_k}=-\frac{\partial f_{ij}}{\partial q_k}g_{ij}, \tag{4·13}$$

it follows that

$$\frac{\partial f_{ij}}{\partial q_k}\frac{\partial g_{ij}}{\partial q_l}=\frac{\partial f_{ij}}{\partial q_l}\frac{\partial g_{ij}}{\partial q_k}. \tag{4·14}$$

Then it is easy to see that

$$R_{ia}=0\,. \tag{4·15}$$

The third term of (4·10) vanishes because $\delta q_i=0$ at the boundary. Substituting (4·12) and (4·15) into (4·10), one gets

$$\int_{t_1}^{t_2}\left[\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_a}-\frac{\partial L}{\partial q_a}-\frac{\partial Z}{\partial q_a}-\frac{1}{4}\frac{\partial f_{ik}}{\partial q_a}\frac{\partial}{\partial q_k}\left(f_{jl}\frac{\partial g_{ij}}{\partial q_l}\right)\right]\delta q_a=0\,. \tag{4·16}$$

Thus the modified Euler-Lagrange equation (2·20) is obtained.

As the consequence, if one deals with δq_i and $\delta \dot{q}_i$ as q-numbers and uses the commutation relations (4·5) to (4·7), the principle of the least action is valid also in the case of velocity dependent potential. The correct Hamiltonian, whose eigenvalue is an energy of a system, is H of (2·14). Then the canonical equation of motion with this H is same as the modified Euler-Lagrange equation derived from the variation principle. In this formalism, everything is consistent.

§ 5. Discussion

As was pointed out in § 3, the ordinary definition of canonical momentum and commutation relations are not independent assumptions if the canonical equation of motion is required. It is, however, left as an open question whether it is possible or not to construct a consistent formulation by modifying both of the assumptions and by defining the Hamiltonian in the ordinary way: $H=\frac{1}{2}\{p_i, \dot{q}_i\}-L$.

Since the variation principle is adequate also in the case of the velocity-dependent potential, if the Lagrangean is invariant under a continuous transformation, a conservation law of the associated physical quantity follows from the variation method keeping an ordering of operators.

It would be worthwhile to notice that formulation of the non-linear chiral invariant Lagrangean[3] should be re-examined from the viewpoint of our argument.

The quantization of the gravitational field also has a relation to our theory, though, in this case, there is no transformation to the standard form.

The argument in this paper is valid only in the special case where the transformation to the standard form exists. Therefore, it remains to build up a consistent theory in general cases where no such transformations exist. The main problem is to set up commutation relations of δq_i and $\delta \dot{q}_i$ with q_j and $\dot{q}_j$ without resorting to the Q-system. The i-j symmetric part of $[\dot{q}_i, \delta q_j]$ and the i-j anti-symmetric part of $[\dot{q}_i, \delta \dot{q}_j]$ can be found, as was noticed in § 4, from the commutators $[\dot{q}_i, q_j]$ and $[\dot{q}_i, \dot{q}_j]$, respectively. If one disregards, therefore, the first form of Z (2·16a) and takes only the form (2·16b) throughout the theory, one can have the consistent theory by employing the commutators (4·5) to (4·7). Needless to say, it should be examined whether another possibility exists or not. Anyway, however, the other formulation, if possible, has to include the one extended in this paper as the special case.

Appendix A

Derivation of relations between q_i and Q_α

Before calculating Z, it is convenient to obtain relations between q_i and Q_α which are useful in the derivation of Z and commutators of δq_i and $\delta \dot{q}_i$ in Appendix B.

From (2·8) and

$$\frac{\partial Q_\alpha}{\partial q_i}\frac{\partial q_i}{\partial Q_\beta}=\delta_{\alpha\beta}\,, \qquad \frac{\partial q_i}{\partial Q_\alpha}\frac{\partial Q_\alpha}{\partial q_j}=\delta_{ij}\,, \tag{A·1}$$

it follows that

$$\frac{\partial q_i}{\partial Q_\alpha}=f_{ij}\frac{\partial Q_\alpha}{\partial q_j}\,, \qquad \frac{\partial Q_\alpha}{\partial q_i}=g_{ij}\frac{\partial q_j}{\partial Q_\alpha} \tag{A·2}$$

and

$$\frac{\partial Q_\alpha}{\partial q_i}\frac{\partial Q_\alpha}{\partial q_j}=g_{ij}\,, \qquad \frac{\partial q_i}{\partial Q_\alpha}\frac{\partial q_j}{\partial Q_\alpha}=f_{ij}\,. \tag{A·3}$$

Differentiation of (A·3) with respect to q_k gives

$$\frac{\partial^2 Q_\alpha}{\partial q_i \partial q_k}\frac{\partial Q_\alpha}{\partial q_j}+\frac{\partial Q_\alpha}{\partial q_i}\frac{\partial^2 Q_\alpha}{\partial q_j \partial q_k}=\frac{\partial g_{ij}}{\partial q_k}\,. \tag{A·4}$$

Integrating the second term of (A·4) by part, one finds

$$\frac{\partial^2 Q_\alpha}{\partial q_i \partial q_k}\frac{\partial Q_\alpha}{\partial q_j}-\frac{\partial^2 Q_\alpha}{\partial q_i \partial q_j}\frac{\partial Q_\alpha}{\partial q_k}=\frac{\partial g_{ij}}{\partial q_k}-\frac{\partial g_{ik}}{\partial q_j} \tag{A·5}$$

and then

$$\frac{\partial^2 Q_\alpha}{\partial q_i \partial q_k}\frac{\partial Q_\alpha}{\partial q_j}=\frac{1}{2}\left(\frac{\partial g_{ij}}{\partial q_k}-\frac{\partial g_{ik}}{\partial q_j}+\frac{\partial g_{jk}}{\partial q_i}\right)\equiv\frac{1}{2}G_{ijk}\,, \tag{A·6}$$

where

$$G_{ijk}=G_{kji}\,. \tag{A·7}$$

Analogously one has

$$\frac{\partial^2 q_i}{\partial Q_\alpha \partial Q_\beta}\frac{\partial q_j}{\partial Q_\alpha}+\frac{\partial q_i}{\partial Q_\alpha}\frac{\partial^2 q_j}{\partial Q_\alpha \partial Q_\beta}=\frac{\partial f_{ij}}{\partial Q_\beta}=\frac{\partial f_{ij}}{\partial q_k}f_{kl}\frac{\partial Q_\beta}{\partial q_l}\,, \tag{A·8}$$

$$\frac{\partial^2 q_i}{\partial Q_\alpha \partial Q_\beta}\frac{\partial q_j}{\partial Q_\alpha}-\frac{\partial q_i}{\partial Q_\alpha}\frac{\partial^2 q_j}{\partial Q_\alpha \partial Q_\beta}=-\left(f_{ik}\frac{\partial f_{jl}}{\partial q_k}-f_{jk}\frac{\partial f_{il}}{\partial q_k}\right)\frac{\partial Q_\beta}{\partial q_l} \tag{A·9}$$

and

$$\frac{\partial^2 q_i}{\partial Q_\alpha \partial Q_\beta}\frac{\partial q_j}{\partial Q_\alpha}=-\frac{1}{2}f_{ik}f_{jl}G_{lkm}\frac{\partial q_m}{\partial Q_\beta}\,. \tag{A·10}$$

In the step from (A·8) and (A·9) to (A·10), uses have been made of (A·2) and the relation

$$f_{ik}f_{jl}\frac{\partial g_{kl}}{\partial q_m}=-\frac{\partial f_{ij}}{\partial q_m}\,. \tag{A·11}$$

Differentiating the first equation of (A·2) and using (A·6), one gets

$$\frac{\partial^2 q_i}{\partial q_j \partial Q_\alpha}=-\frac{1}{2}f_{ik}G_{jkl}\frac{\partial q_l}{\partial Q_\alpha}\,. \tag{A·12}$$

Similarly from (A·2) with the help of (A·6) and (A·11), it follows that

$$\frac{\partial^2 q_i}{\partial Q_\alpha{}^2}=\frac{\partial f_{ij}}{\partial q_j}+\frac{1}{2}f_{ij}f_{kl}\frac{\partial g_{kl}}{\partial q_j}\equiv F_i\,. \tag{A·13}$$

It will be worthwhile to note that $(\partial/\partial Q_\alpha)\delta=\delta(\partial/\partial Q_\alpha)$ because, noting $\delta P_\alpha=\delta\dot{Q}_\alpha=c$-number,

$$-i\delta\frac{\partial A(Q)}{\partial Q_\alpha}=\delta[P_\alpha, A(Q)]=[\delta P_\alpha, A(Q)]+[P_\alpha, \delta A(Q)]=-i\frac{\partial}{\partial Q_\alpha}\delta A(Q)\,, \tag{A·14}$$

while $(\partial/\partial q_i)\delta\neq\delta(\partial/\partial q_i)$. In fact, one finds

$$\frac{\partial \delta q_i}{\partial q_j}=\frac{\partial}{\partial q_j}\left(\frac{\partial q_i}{\partial Q_\alpha}\delta Q_\alpha\right)=-\frac{1}{2}f_{ik}G_{jkl}\delta q_l\,. \tag{A·15}$$

Appendix B

Derivation of Z and commutators of δq_i and $\delta \dot{q}_i$

Although the first expression of Z (2·16a) was obtained in I, a simpler derivation is presented here. Since the two expressions of Z in (2·15) lead to the same results (2·16a) and (2·16b), the second one of (2·15) will be employed in the following derivation. Then one gets

$$4Z = -\frac{\partial^2 q_i}{\partial q_j \partial Q_\alpha}\frac{\partial^2 q_j}{\partial q_i \partial Q_\alpha} = -\frac{\partial}{\partial q_i}\left(\frac{\partial^2 q_i}{\partial q_j \partial Q_\alpha}\frac{\partial q_j}{\partial Q_\alpha}\right) + \frac{\partial^3 q_i}{\partial q_i \partial q_j \partial Q_\alpha}\frac{\partial q_j}{\partial Q_\alpha}$$

$$= -\frac{\partial}{\partial q_i}\left(\frac{\partial^2 q_i}{\partial Q_\alpha{}^2}\right) + \frac{\partial}{\partial Q_\alpha}\left(\frac{\partial^2 q_i}{\partial q_i \partial Q_\alpha}\right). \tag{B·1}$$

With the aid of (A·12) and (A·13), this becomes

$$4Z = -\frac{\partial F_i}{\partial q_i} - \frac{1}{2} f_{ij}\frac{\partial g_{ij}}{\partial q_k} F_k - \frac{1}{2} f_{kl}\frac{\partial}{\partial q_k}\left(f_{ij}\frac{\partial g_{ij}}{\partial q_l}\right), \tag{B·2}$$

which immediately reduces to (2·16a).

On the other hand, if one applies (A·12) to the first expression of Z in (B·1), one has

$$4Z = -\frac{1}{4} f_{ik} G_{jkl}\frac{\partial q_l}{\partial Q_\alpha} f_{jm} G_{imn}\frac{\partial q_n}{\partial Q_\alpha}$$

$$= -\frac{1}{4} f_{ik} f_{jm} f_{ln} G_{jkl} G_{imn}\,.$$

Noting $G_{imn} = G_{nmi}$ and $f_{ij} = f_{ji}$, one can easily see that $f_{ik} f_{ln} G_{imn}$ is symmetric with respect to k and l. Then G_{jkl} reduces to $\partial g_{kl}/\partial q_j$ and hence

$$4Z = \frac{1}{4}\frac{\partial f_{in}}{\partial q_j} f_{jm} G_{imn}$$

$$= -\frac{1}{4} f_{jk}\frac{\partial f_{il}}{\partial q_j}\frac{\partial g_{il}}{\partial q_k} + \frac{1}{2} f_{jk}\frac{\partial f_{il}}{\partial q_j}\frac{\partial g_{kl}}{\partial q_i}, \tag{B·3}$$

where (A·11) has been used.

Next let us calculate the commutators of δq_i and $\delta \dot{q}_i$. Here δQ_α and $\delta \dot{Q}_\alpha$ are assumed to be c-numbers. (4·5) is obvious. Using (4·1) and the expression

$$\dot{q}_i = \frac{1}{2}\left\{\dot{Q}_\alpha, \frac{\partial q_i}{\partial Q_\alpha}\right\}, \tag{B·4}$$

one finds, with the aid of (A·10)

$$[\dot{q}_i, \delta q_j] = -i\frac{\partial^2 q_j}{\partial Q_\alpha \partial Q_\beta}\frac{\partial q_i}{\partial Q_\alpha}\delta Q_\beta = \frac{i}{2} f_{ik} f_{jl} G_{klm}\delta q_m\,. \tag{B·5}$$

Similarly (4·2) and (A·10) give

$$[q_i, \delta \dot{q}_j] = [q_i, \dot{Q}_\alpha]\frac{\partial^2 q_j}{\partial Q_\alpha \partial Q_\beta}\delta Q_\beta = i\frac{\partial q_i}{\partial Q_\alpha}\frac{\partial^2 q_j}{\partial Q_\alpha \partial Q_\beta}\delta Q_\beta = -\frac{i}{2} f_{ik} f_{jl} G_{klm}\delta q_m\,. \tag{B·6}$$

Finally let us obtain $[\dot{q}_i, \delta \dot{q}_j]$. With (4·2) and (B·4) one has

$$[\dot{q}_i, \delta \dot{q}_j] = -i\frac{\partial q_i}{\partial Q_\alpha}\frac{\partial^2 q_j}{\partial Q_\alpha \partial Q_\beta}\delta \dot{Q}_\beta - \frac{i}{2}\left\{\delta\left(\frac{\partial^2 q_j}{\partial Q_\alpha \partial Q_\beta}\right)\frac{\partial q_i}{\partial Q_\alpha} - \delta\left(\frac{\partial q_j}{\partial Q_\alpha}\right)\frac{\partial^2 q_i}{\partial Q_\alpha \partial Q_\beta}, \dot{Q}_\beta\right\}$$

$$= -\frac{i}{2}\delta\left\{\frac{\partial q_i}{\partial Q_\alpha}\frac{\partial^2 q_j}{\partial Q_\alpha \partial Q_\beta}, \dot{Q}_\beta\right\}$$

$$+\frac{i}{2}\left\{\delta\left(\frac{\partial q_i}{\partial Q_\alpha}\right)\frac{\partial^2 q_j}{\partial Q_\alpha \partial Q_\beta} + \delta\left(\frac{\partial q_j}{\partial Q_\alpha}\right)\frac{\partial^2 q_i}{\partial Q_\alpha \partial Q_\beta}, \dot{Q}_\beta\right\}. \tag{B·7}$$

For the first term, one may rewrite, by using (A·10), as

$$\left\{\frac{\partial q_i}{\partial Q_\alpha}\frac{\partial^2 q_j}{\partial Q_\alpha \partial Q_\beta}, \dot{Q}_\beta\right\} = \left\{\frac{\partial q_i}{\partial Q_\alpha}\frac{\partial^2 q_j}{\partial Q_\alpha \partial Q_\beta}\frac{\partial Q_\beta}{\partial q_k}, \dot{q}_k\right\} = -\frac{1}{2}\{f_{il} f_{jm} G_{lmk}, \dot{q}_k\}. \tag{B·8}$$

For the second term, one obtains, using (A·14), (A·10) and (A·15),

$$\left\{\delta\left(\frac{\partial q_i}{\partial Q_\alpha}\right)\frac{\partial^2 q_j}{\partial Q_\alpha \partial Q_\beta}, \dot{Q}_\beta\right\} = \left\{\frac{\partial \delta q_i}{\partial Q_\alpha}\frac{\partial^2 q_j}{\partial Q_\alpha \partial Q_\beta}\frac{\partial Q_\beta}{\partial q_k}, \dot{q}_k\right\}$$

$$= \left\{\frac{\partial \delta q_i}{\partial q_l}\frac{\partial q_l}{\partial Q_\alpha}\frac{\partial^2 q_j}{\partial Q_\alpha \partial Q_\beta}\frac{\partial Q_\beta}{\partial q_k}, \dot{q}_k\right\} = \frac{1}{4}\{f_{im} f_{jr} f_{ls} G_{lmn} G_{srk} \delta q_n, \dot{q}_k\}. \tag{B·9}$$

Substitution of (B·8) and (B·9) into (B·7) leads us to (4·7).

References

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