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Comments on Transition from Classical to Quantum Mechanics in Generalized Coordinates via the Covariant Derivative

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Many people have asked me in connection with my previous articles why one could not make a transition from classical to quantum theory in generalized coordinates via the covariant derivative. I will show why one cannot, in this note, and also show an interesting connection between the covariant derivative operator and the 'measurable' generalized momentum operator.

Consider the *classical* Hamiltonian of a free particle in generalized coordinates, *H*. *H* is given by (Brillouin, 1949)

$$H = \sum_{m,n} g^{mn} p_m p_n \qquad (1)$$

where p_m is the canonical momentum and g^{mn} is a function of the generalized coordinates $\{q_i\}$. In *Cartesian* coordinates, in order to produce the *quantum* Hamiltonian operator, one merely substitutes for p_m, $p_m = -i\hbar\,\partial/\partial x_m$, into equation (1). It would seem that in *generalized* coordinates, in order to produce the quantum Hamiltonian operator, one would substitute in equation (1), $p_m = -i\hbar D/Dq_m$, where D/Dq_m denotes the covariant derivative† given by (Brillouin, 1949)

$$\frac{D}{Dq_m} = \frac{\partial}{\partial q_m} - \sum_n \Gamma^h_{in}\left(= \frac{\partial}{\partial q_m} - \tfrac{1}{2}\sum_{i,j} g^{ij}\frac{\partial g_{ij}}{\partial q_m}\right)$$

where Γ^h_{ih} is the familiar Christoffel symbol used in Riemannian geometry. It is both interesting and instructive to note that no matter what ordering

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† It is seen from Gruber (1971) that one cannot simply substitute for p_m, the operator $p_m = -i\hbar\,\partial/\partial q_m$.

we choose for the operators D/Dq_m, D/Dq_n, and g^{mn} in equation (1), that is

$$H_Q = \sum_{m,n} g^{mn}\frac{D}{Dq_m}\frac{D}{Dq_n} \quad \text{or} \quad H_Q = \sum_{m,n}\frac{D}{Dq_m} g^{mn}\frac{D}{Dq_n}, \text{etc.}$$

even if we take Hermitian parts of H_Q, we will not arrive at the correct quantum Hamiltonian, which is a transformation from $-\hbar^2\nabla^2$ to generalized coordinates. For example if

$$H_Q = \text{Hermitian part of}\left\{-\hbar^2\sum_{m,n} g^{mn}\frac{D}{Dq_m}\frac{D}{Dq_n}\right\}$$

we find

$$H_Q = H' - \tfrac{1}{2}\sum_{m,n}\frac{1}{g}\frac{\partial}{\partial q_m}\left[\frac{\partial g}{\partial q_n} g^{nm}\right] \qquad (g^{-1} = \sqrt{\det g^{ik}})$$

The correct quantum Hamiltonian H' is given by (Blokhinstev, 1964)

$$H' = \sum_{m,n} g^{mn}\frac{\partial^2}{\partial q_m\,\partial q_n} + \frac{\partial g^{mn}}{\partial q_n}\frac{\partial}{\partial q_m} + \frac{1}{g}\frac{\partial g}{\partial q_n} g^{mn}\frac{\partial}{\partial q_m}$$

Thus there is an extra term in H_Q, namely, the term

$$-\tfrac{1}{2}\sum_{m,n}\frac{1}{g}\frac{\partial}{\partial q_m}\left[\frac{\partial g}{\partial q_n} g^{nm}\right]$$

The interesting and rather mystifying thing is that the 'measurable' momentum operator which is the Hermitian part of $p_m = -i\hbar\,\partial/\partial q_m$ (see Gruber, 1972a), is the Hermitian part of the covariant derivative operator.

Proof: In our previous notation (Gruber, 1972a, b), the Hermitian part of $-i\hbar D/Dq_i$, that is, $[-i\hbar D/Dq_i]^H$ is given as‡

$$\begin{aligned}\left[-i\hbar\frac{D}{Dq_i}\right]^H &= \frac{1}{2}\left[\left(-i\hbar\frac{D}{Dq_i}\right)^\dagger - i\hbar\frac{D}{Dq_i}\right]\\ &= \frac{1}{2}\left[\left(p_i + i\hbar\frac{1}{g}\frac{\partial g}{\partial q_i}\right)^\dagger + \left(p_i + i\hbar\frac{1}{g}\frac{\partial g}{\partial q_i}\right)\right]\\ &= \frac{1}{2}\left[p_i{\dagger} - i\hbar\frac{1}{g}\frac{\partial g}{\partial q_i} + p_i + i\hbar\frac{1}{g}\frac{\partial g}{\partial q_i}\right]\\ &= \tfrac{1}{2}(p_i{\dagger} + p_i) = (p_i)^H\end{aligned}$$

Q.E.D.

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‡ Here, $A\dagger$ denotes adjoint of A.