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On the Transition from Classical to Quantum Mechanics in Generalized Coordinates

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The classical Hamiltonian in generalized coordinates is given as $H = \frac{1}{2}\sum_{i,k} p_i g^{ik} p_k$. *We show that there is no operator of the form* $P_i = -iA(q_i)(\partial/\partial q_i) + G_i(q_i)$ *(note that the Hermitian momentum operator* P_i^H *is of this form) such that the quantum Hamiltonian operator* H_Q *is given as* $H_Q = \frac{1}{2}\sum_{i,k} P_i g^{ik} P_k$ or $\frac{1}{2}\sum_{i,k} g^{ik} P_i P_k$, *etc. In order to maintain a direct transition of this sort from classical to quantum theory, using the classical Hamiltonian as a starting point, we must rely on our previous prescriptions, writing the quantum Hamiltonian as* $H_Q = \frac{1}{2}\sum_{i,k} P_i^{\dagger} g^{ik} P_k$, *where* $P_i^{\dagger}$ denotes *the adjoint of the operator* $P_i = -i\hbar\, \partial/\partial q_i$.

Consider the classical Hamiltonian H in generalized coordinates,[1]

$$H = \tfrac{1}{2} \sum_{i,k} p_i g^{ik} p_k \tag{1}$$

where p_i and g^{ik} are, respectively, the canonical momentum and the contravariant metric tensor, which is dependent on the generalized coordinates $\{q_i\}$.

To investigate the transition to quantum mechanics, we might substitute a general operator of the form

$$P_i = -iA(q_i) \frac{\partial}{\partial q_i} + G_i(q_i) \tag{2}$$

for p_i in Eq. (1), keeping g^{ik} the same function of $\{q_i\}$. We would get for the quantum Hamiltonian operator H_Q,[2]

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[2] Note that we use the form $H_Q = \frac{1}{2}\sum_{i,k} p_i g^{ik} p_k$ here. We could have chosen any other ordering, such as $H_Q = \frac{1}{2}\sum_{i,k} p_i p_k g^{ik}$, etc. and we would obtain the same results.

$$\begin{aligned} H_Q &= \frac{1}{2}\sum_{i,k}\left(-iA\frac{\partial}{\partial q_i} + G_i\right) g^{ik} \left(-iA\frac{\partial}{\partial q_k} + G_k\right) \\ &= \frac{1}{2}\sum_{i,k}\left[-iA\frac{\partial g^{ik}}{\partial q_i}\left(-iA\frac{\partial}{\partial q_k}\right)\right. \\ &\quad - iA\frac{\partial}{\partial q_i}(g^{ik}G_k + G_i g^{ik}\left(-iA\frac{\partial}{\partial q_k}\right) + G_i g^{ik} G_k \end{aligned} \tag{3}$$

We know from Refs. 1 and 2 that the correct form of the quantum Hamiltonian operator H_Q is given as

$$H_Q = \frac{1}{2}\sum_{i,k}\left(-i\frac{\partial}{\partial q_i} - i\frac{1}{g}\frac{\partial g}{\partial q_i}\right) g^{ik}\left(-i\frac{\partial}{\partial q_k}\right) \tag{4}$$

where g is the square root of the determinent $|g_{ik}|$. Comparing Eqs. (3) and (4) and equating coefficients of $(\partial/\partial q_i)(\partial/\partial q_k)$, $\partial/\partial q_i$, etc., we find that

$$A(q_i) = 1, \qquad G_i(q_i) = \frac{1}{2}\frac{1}{g}\frac{\partial g}{\partial q_i} \tag{5}$$

and

$$\sum_{i,k} G_i G_k g^{ik} = \sum_{i,k}\left(\frac{1}{4}\right)\left(\frac{1}{g^2}\right)\left(\frac{\partial g}{\partial q_i}\right)\left(\frac{\partial g}{\partial q_k}\right) g^{ik} = 0 \tag{6}$$

Note that obviously not every coordinate system will satisfy Eq. (6); thus we have shown that there is in general no operator of the form $P_i = -iA(q_i)(\partial/\partial q_i) + G_i(q_i)$ which may be substituted in the classical Hamiltonian given by Eq. (1) to produce the correct quantum Hamiltonian operator. Note that since the Hermitian momentum operator P_i^H is given as[2]

$$P_i^H = -i\frac{\partial}{\partial q_i} - \frac{1}{2}\frac{1}{g}\frac{\partial g}{\partial q_i} \tag{7}$$

and is of the form of P_i given in Eq. (2), the Hermitian momentum operator cannot be used to produce the transition from classical to quantum mechanics in the method described above. If we want a direct transition from the classical generalized Hamiltonian to the quantum generalized Hamiltonian, we must rely on our previous prescriptions,[2,3] where we find

$$H_Q = \tfrac{1}{2}\sum_{i,k} P_i^{\dagger} g^{ik} P_k$$

where $P_i^{\dagger}$ is the adjoint of the operator P_i.

In passing, it is interesting to note that, specifically, no combination of ordering the operators P_i^{H}, g^{ik}, and P_k^{H} such as

$$H_Q = \frac{1}{2} \sum_{i,k} P_i^{\mathrm{H}} g^{ik} P_k^{\mathrm{H}} \quad \text{or} \quad \frac{1}{2} \sum_{i,k} P_i^{\mathrm{H}} P_k^{\mathrm{H}} g^{ik}, \quad \text{etc.}$$

will produce the correct quantum Hamiltonian operator.

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