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Quantization in Generalized Coordinates III—Lagrangian Formulation

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Abstract

It is shown that if one incorporates the generalized coordinate quantum velocities $\dot{q}^i$ as given by $\dot{q}^i = i[H,q^i]$ ($\hbar = 1$) into the generalized classical Lagrangian for a free particle (the total energy), $L = \frac{1}{2}\dot{q}^i g_{ik}\dot{q}^k$, one does not obtain (no matter what ordering of the operators $\dot{q}^i$, $\dot{q}^k$, and g_{ik} we choose) the correct quantum Lagrangian operator which is a transformation from $-\frac{1}{2}\nabla^2$ to generalized coordinates (Gruber, 1971, 1972). $\dot{q}^i$ as given by $\dot{q}^i = i[H,q^i]$ turns out to be the Hermitian part of a more generalized operator which we call the total generalized velocity operator similar to the notation in our previous articles (Gruber, 1971, 1972). This total velocity operator really determines the fundamental structure governing our system in the Lagrangian formulation. We show that it is through the total velocity operator that we make the transition from classical to quantum mechanics and through our procedure we arrive at the correct quantum Lagrangian operator.

1. *Introduction*

In two previous articles, I (Gruber, 1971) and II (Gruber, 1972), I have shown a prescription for the transition of classical quantities to their corresponding quantum operators in generalized coordinates. These prescriptions deal with, representing quantum mechanically, operators in generalized coordinates corresponding to classical functions of generalized momenta and coordinates, such as the Hamiltonian of the system. Difficulty arises when one tries to represent in generalized coordinates quantum mechanical operators corresponding to functions of generalized velocities and coordinates. For example, consider the following: The total energy of a free particle (the Lagrangian) expressed in generalized coordinates is classically given by Brillouin (1949) (throughout this article, repeated indices denote Einstein summation)

$$L = \tfrac{1}{2} g_{ik}\dot{q}^i\dot{q}^k \tag{1.1}$$

where g_{ik} are functions of the generalized coordinates and $\dot{q}^i$ is the generalized velocity. Now if one substitutes the operator $\dot{q}^i$ given by the familiar equation†

$$\dot{q}^i = i[H, q^i] = i(Hq^i - q^i H) \tag{1.2}$$

into the Lagrangian of equation (1.1), no matter what the ordering we choose for $\dot{q}^i$, $\dot{q}^k$, and g_{ik} (that is, if $L = \frac{1}{2}\dot{q}^i g_{ik} \dot{q}^k$ or $L = \frac{1}{2}\dot{q}^i \dot{q}^k g_{ik}$, etc.) we will *not* arrive at the correct quantum Lagrangian operator which is given as (Gruber, 1972)

$$L = -\frac{1}{2}\frac{1}{g}\frac{\partial}{\partial q^i}\left(g g^{ik} \frac{\partial}{\partial q^k}\right) \tag{1.3}$$

where g is the Jacobian $|\partial x^i/\partial q^k|$ (Sokolnikoff, 1951) of the transformation from Cartesian to generalized coordinates and g^{ik} is the contravariant metric tensor (Gruber, 1972).

In the following sections we will proceed to find what the fundamental velocity operator is and how to incorporate it into the classical generalized Lagrangian to get the correct quantum-mechanical Lagrangian operator. We will also show just what the real significance of the operator $\dot{q}^i$, given as $\dot{q}^i = i[H, q^i]$, is.

2. *Representation of Generalized Velocities in Quantum Theory*

Consider the classical Lagrangian expressed in generalized coordinates:

$$L = \tfrac{1}{2} g_{ik} \dot{q}^i \dot{q}^k \tag{1.1}$$

The generalized classical momentum p_i is given as

$$p_i = \frac{\partial L}{\partial \dot{q}^i} = \dot{q}^k g_{ki} \tag{2.1}$$

Multiplying both sides of equation (2.1) by g^{ij}, we obtain (classically)

$$\dot{q}^j = g^{ij} p_i \tag{2.2}$$

This is because

$$g_{ik} g^{kj} = \delta_i^{\ j} \begin{cases} = 0, & j \neq i \\ = 1, & j = i \end{cases}$$

Now, quantum-mechanically, we postulate (Gruber, 1971, 1972) that $p_i \to -i\partial/\partial q^i$ ($\hbar = 1$). Thus we note that quantum-mechanically, $\dot{q}^j$ can be written as either

$$\dot{q}_{\text{I}}^{\,j} = g^{ij} p_i \tag{2.3}$$

or as

$$\dot{q}_{\text{II}}^{\,j} = p_i g^{ij} \tag{2.4}$$

since p_i and g^{ij} do not commute.

† Here, H is the Hamiltonian given by $H = -\frac{1}{2}\nabla^2 = \frac{1}{2}p^i g^{ik} p_k$ (Gruber, 1971, 1972).

Let us compute what $\dot{q}^i$ is, as given by equation (1.2). Since (Gruber, 1972) $H = \frac{1}{2}p_i^\dagger g^{ik} p_k$ (where as in the notation of Gruber (1971, 1972) $p_i^\dagger$ denotes the adjoint of p_i),

$$\dot{q}^i = i[H, q^i] = i[\tfrac{1}{2}p_j^\dagger g^{jk} p_k, q^i]$$
$$= i(\tfrac{1}{2}p_j^\dagger g^{jk} p_k q^i - \tfrac{1}{2}q^i p_j^\dagger g^{jk} p_k)$$

Since $[q^i, p_j] = [q^i, p_j^\dagger] = i\delta_i{}^j$, the former equation becomes

$$\dot{q}^i = \tfrac{1}{2}(p_k^\dagger g^{ik} + g^{ik} p_k) \tag{2.5}$$

Now because the Hermitian part of $\dot{q}_\mathrm{I}{}^j$, $(\dot{q}_\mathrm{I}{}^j)^H$, is given as

$$(\dot{q}_\mathrm{I}{}^j)^H = \frac{(\dot{q}_\mathrm{I}{}^j)^\dagger + (\dot{q}_\mathrm{I}{}^j)}{2}$$

we have from equation (2.3) that

$$(\dot{q}_\mathrm{I}{}^j)^H = \frac{p_i^\dagger g^{ij} + g^{ij} p_i}{2} \tag{2.6}$$

Thus $(\dot{q}_\mathrm{I}{}^j)^H$ is just $\dot{q}^j$ given by equation (2.5) which was derived by equation (1.2). For the Hermitian part of $(\dot{q}_\mathrm{II}^j)$, $(\dot{q}_\mathrm{II}^j)^H$, we have

$$(\dot{q}_\mathrm{II}^j)^H = \frac{(\dot{q}_\mathrm{II}^j)^\dagger + (\dot{q}_\mathrm{II}^j)}{2} = \frac{g^{ij} p_i^\dagger + p_i g^{ij}}{2}$$

Since $p_i^\dagger = p_i - iF_i$ where $F_i = (1/g)(\partial g/\partial q^i)$ (Gruber, 1971, 1972), we have

$$(\dot{q}_\mathrm{II}^j)^H = \frac{g^{ij}(p_i - iF_i) + p_i g^{ij}}{2}$$
$$= \frac{g^{ij} p_i - iF_i g^{ij} + p_i g^{ij}}{2}$$

Now using equation (2.6) we have

$$(\dot{q}_\mathrm{I}{}^j)^H = \frac{(p_i - iF_i) g^{ij} + g^{ij} p_i}{2}$$
$$= \frac{p_i g^{ij} - iF_i g^{ij} + g^{ij} p_i}{2}$$

Thus it is seen that $(\dot{q}_\mathrm{I}{}^j)^H = (\dot{q}_\mathrm{II}^j)^H$. It can be similarly shown that

$$[(\dot{q}_\mathrm{I}{}^j)^\dagger]^H = [(\dot{q}_\mathrm{II}^j)^\dagger]^H = (\dot{q}_\mathrm{I}{}^j)^H$$

Thus we find that

$$(\dot{q}_\mathrm{I}{}^j)^H = (\dot{q}_\mathrm{II}^j)^H = [(\dot{q}_\mathrm{I}{}^j)^\dagger]^H = [(\dot{q}_\mathrm{II}^j)^\dagger]^H = i[H, q^j] \tag{2.7}$$

and therefore the operator $\dot{q}^i$ in equation (1.2) really corresponds to the Hermitian part of a more fundamental operator, the 'total' velocity operator, $\dot{q}_\mathrm{I}{}^j$ or $\dot{q}_\mathrm{II}^j$ (or $(\dot{q}_\mathrm{I}{}^j)^\dagger$ or $(\dot{q}_\mathrm{II}^j)^\dagger$).

3. *Correct Incorporation of the Total Velocity Operators into the Lagrangian*

The following is very analogous to what is achieved by Gruber (1972, Section 2) with the Hamiltonian.

Since the classical Lagrangian should be positive-definite, we write the Lagrangian L given by equation (1.1) as

$$L = \tfrac{1}{2}(\dot{q}^i)^* g_{ik}\dot{q}^k \tag{3.1}$$

where $(\dot{q}^i)^*$ denotes the complex-conjugate of $\dot{q}^i$. This suggests that the quantum operator corresponding to the classical Lagrangian be

$$L_I = \tfrac{1}{2}(\dot{q}_I{}^i)^\dagger g_{ik}\dot{q}_I{}^k \tag{3.2}$$

or

$$L_{II} = \tfrac{1}{2}(\dot{q}_{II}^i)^\dagger g_{ik}\dot{q}_{II}^k \tag{3.3}$$

From equation (2.3) we find that

$$\begin{aligned} L_I &= \tfrac{1}{2}p_m^\dagger g^{im} g_{ik} g^{ks} p_s \\ &= \tfrac{1}{2}p_m^\dagger \delta_k{}^m g^{ks} p_s \\ &= \tfrac{1}{2}p_k^\dagger g^{ks} p_s \end{aligned}$$

which is just the quantum Lagrangian operator for a free particle (the Hamiltonian operator for a free particle) derived in Gruber (1972).

For L_{II} we have

$$\begin{aligned} L_{II} &= \tfrac{1}{2}(\dot{q}_{II}^i)^\dagger g_{ik}\dot{q}_{II}^k \\ &= \tfrac{1}{2}g^{im} p_m^\dagger g_{ik} p_s g^{ks} \end{aligned}$$

Since

$$[g^{ik}, p_k^\dagger] = i\frac{\partial g^{ik}}{\partial q^k} = [g^{ik}, p_k]$$

we find

$$L_{II} = \tfrac{1}{2}p_m^\dagger g^{ms} p_s - \frac{1}{2}\frac{\partial g^{ms}}{\partial q^s}\left(\frac{1}{g}\frac{\partial g}{\partial q^m}\right) - \frac{1}{2}\frac{\partial^2 g^{ms}}{\partial q^m \partial q^s} - \frac{1}{2}\frac{\partial g^{il}}{\partial q^i}\frac{\partial g^{ms}}{\partial q^s} g_{lm} \tag{3.4}$$

For spherical polar coordinates and polar coordinates or for transformations where g^{ik} is independent of q^k, the last three terms in equation (3.4) vanish and L_{II} becomes our quantum Lagrangian operator for a free particle (the Hamiltonian for a free particle). Since L_I (rather than L_{II}) was derived as the quantum Lagrangian in an unrestricted (general) way, this suggests that $\dot{q}_I{}^j$ rather than $\dot{q}_{II}^j$ be our total generalized coordinates velocity operator.

4. *Comments and Discussion*

We have shown that there exists a total velocity operator in generalized coordinates, $\dot{q}_I{}^i = g^{ij}p_j = -ig^{ij}\partial/\partial q^j$, such that the Hermitian part of $(\dot{q}_I{}^i)$, $(\dot{q}_I{}^i)^H$, is the 'measurable' velocity operator as derived from the familiar equation $\dot{q}^i = i[H, q^i]$. If the classical Lagrangian in generalized coordinates, L, is written as $L = \frac{1}{2}(\dot{q}^i)^* g_{ik} \dot{q}^k$ (to preserve positive-definiteness) where $(\dot{q}^i)^*$ denotes the complex-conjugate of $\dot{q}^i$, the quantum Lagrangian operator is written as $L = \frac{1}{2}(\dot{q}_1^i)^\dagger g_{ik} \dot{q}_1^k$ analogous to the prescriptions for the Hamiltonian operator in Gruber (1972). Thus the operator $\dot{q}^i = i[H, q^i]$ is *not* the fundamental velocity operator and quantum prescriptions must be derived from $\dot{q}_1^i$ and its adjoint $(\dot{q}_1^i)^\dagger$ as shown in this article.

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