International Journal of Theoretical Physics, Vol. 6, No. 1 (1972), pp. 31–35

Quantization in Generalized Coordinates—II

GARY R. GRUBER

Physics Department, Hofstra University,
Hempstead, Long Island, New York 11550

Received 29 *July* 1971

Abstract

In a previous article (Gruber, 1971), the author considered what the operator form of the generalized canonical momenta was is quantum mechanics. As noted in the article, Pauli (1950), through a different method, found what the generalized momentum operator was also, and both results (the author's and Pauli's) were in agreement. However, the prescription of incorporating the momentum operator into the Hamiltonian, in some cases does not give the correct form of the Hamiltonian operator. In the present article, the author finds exactly how to incorporate the total momentum operator $p_{q_i} = -i\hbar\,\partial/\partial q_i$ into the generalized classical Hamiltonian to get the correct quantum mechanical Hamiltonian operator for all cases. The author also shows a clear-cut way of making the transition from classical observable functions of the canonical momenta to their quantum mechanical operator analogs, in generalized spaces.

1. *Introduction*

In a previous article (Gruber, 1971) by the author, a statement was made concerning the generalized momenta in quantum mechanics. It was stated that the operator form of the generalized momentum p_q, corresponding to the generalized coordinate q, was just the Hermitian part of the operator $-i\hbar\,\partial/\partial q$. We also showed that the Hermitian part of the operator $-i\hbar\,\partial/\partial q, P_q{}^H$, could be expressed in the form

$$P_q{}^H = -i\hbar\frac{1}{g^{1/2}}\frac{\partial}{\partial q}(g^{1/2} \tag{1.1}$$

where g is the Jacobian $|\partial x_i/\partial q_i|$ of the transformation from Cartesian to generalized coordinates $\{q_i\}$. We have noted in the aforementioned article (Gruber, 1971) that Pauli (1950) also arrives at equation (1.1) via a different method. However, much to our surprise, equation (1.1) does not hold†

† When we insert the operator

$$(P_r{}^H)^2 = \left(-i\hbar\frac{1}{\sqrt{r}}\frac{\partial}{\partial r}(\sqrt{r}\right)^2$$

into the two-dimensional classical Hamiltonian we do not get the correct operator form of the Hamiltonian.

when we consider the square of the momentum, $p_r{}^2$, corresponding to the radial coordinate in two dimensions. That is in two dimensions ($g = r$)

$$p_r{}^2 \neq -i\hbar\frac{1}{\sqrt{r}}\frac{\partial}{\partial r}(\sqrt{r}\left(-i\hbar\frac{1}{\sqrt{r}}\frac{\partial}{\partial r}\sqrt{r}\right.$$

In the following sections we proceed to find what the generalized momentum operator 'squared' is for all spaces and show exactly how we incorporate the operators $P_q = -i\hbar\,\partial/\partial q$ into the Hamiltonian to get the correct transition from classical to quantum mechanics.

2. *Representation of Generalized Momenta in Quantum Theory*

In the aforementioned article (Gruber, 1971) we commenced by showing that if one substitutes the operators $p_r \to -i\hbar\,\partial/\partial r$, $p_\theta \to -i\hbar\,\partial/\partial\theta$, and $p_\phi \to -i\hbar\,\partial/\partial\phi$ in the classical Hamiltonian, H, given by

$$H = \frac{p_r{}^2}{2m} + \frac{p_\theta{}^2}{2mr^2} + \frac{p_\phi{}^2}{2mr^2\sin^2\theta}$$

we do not get the correct quantum-mechanical operator corresponding to the Hamiltonian, which is given by

$$H = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{\cot\theta}{r^2}\frac{\partial}{\partial\theta}\right)$$

Thus the question that was asked was 'What is the correct form of the momentum operator in generalized coordinates?' Furthermore we must ask the question (which was only superficially investigated in the previously mentioned articles (Gruber, 1971; Pauli, 1950)), how do we incorporate these operators in the classical Hamiltonian to get the correct quantum mechanical description?

The classical Hamiltonian, H, in generalized coordinates is given by (Brillouin, 1949)

$$H = \frac{1}{2m}\sum_{i,k} p_{q_i} g^{ik} p_{q_k} \tag{2.1}$$

where g^{ik} (a symmetric tensor) is a function of the generalized coordinates q_i and p_{q_i} is the generalized momentum corresponding to the coordinate q_i. m is the mass of the particle. Since H is positive-definite, we will be more general and accurate in writing H as

$$H = \frac{1}{2m}\sum_{i,k} p_{q_i}^{*} g^{ik} p_{q_k} \tag{2.2}$$

(U^* denotes the complex conjugate of U.) We now postulate (as in the author's previous article) that the total quantum-mechanical momentum operator p_{q_i} corresponding to the generalized coordinate q_i is given as

$$p_{q_i} = -i\hbar \frac{\partial}{\partial q_i} \tag{2.3}$$

where the 'measurable' momentum operator is just the Hermitian part of the operator p_{q_i} as noted in Gruber, 1971.

Equation (2.2) suggests that the quantum-mechanical operator corresponding to the Hamiltonian H, be given as

$$H = \frac{1}{2m} \sum_{i,k} p_{q_i}^\dagger g^{ik} p_{q_k} \tag{2.4}$$

where $p_{q_i}^\dagger$ denotes the adjoint of the operator p_{q_i}. This is analogous to $p_{q_i}^*$ being the complex conjugate of p_{q_i} equation (2.2). Note that the 'square' of the momentum operator corresponding to coordinate q_i is just $p_{q_i}^\dagger p_{q_i}$. Also note in general, that the 'true' product of momentum operators $p_{q_i}^\dagger p_{q_k}$ is the Hermitian part, $(p_{q_i}^\dagger p_{q_k})^H$, of the operator $p_{q_i}^\dagger p_{q_k}$. That is, $(p_{q_i}^\dagger p_{q_k})^H = (p_{q_i}^\dagger p_{q_k} + p_{q_k}^\dagger p_{q_i})/2$, since $A^H = (A + A\dagger)/2$ for an operator A. This is analogous to saying that the 'true' physical value of the classical product of momentums, $p_{q_i}^* p_{q_k}$, is the real part of the product $p_{q_i}^* p_{q_k}$.

In the author's previous article, p. 230, we found that the adjoint operator $d_{q_i}^\dagger$ was given as

$$p_{q_i}^\dagger = -i\hbar \left(\frac{\partial}{\partial q_i} + \frac{1}{g} \frac{\partial g}{\partial q_i} \right) \tag{2.5}$$

where g is the Jacobian $|\partial x_i / \partial q_i|$ (Sokolnikoff, 1951) of the transformation of Cartesian to generalized coordinates. Equation (2.5) can be obtained (see Gruber, 1971, pp. 229–230) by first defining the adjoint operator $A\dagger$ through the integral equation

$$\int_{\text{all } V} (A\psi)^* \phi \, dV = \int_{\text{all } V} \psi^* A^\dagger \phi \, dV \tag{2.6}$$

(where $dV = g dq_1 dq_2 dq_3 \ \ldots$; in three dimensions, $dV = dx dy dz = g dq_1 dq_2 dq_3$) and then substituting $A = -i\hbar \partial / \partial q_i = p_{q_i}$ in equation (2.6).

3. *Correct Incorporation of Quantum Mechanical Momenta in Hamiltonian*

We note that the standard way of obtaining the Hamiltonian operator, $-(\hbar^2/2m)\nabla^2 = H$, in generalized coordinates is by performing a coordinate transformation of the operator $-(\hbar^2/2m)\nabla^2$ from Cartesian to generalized coordinates. Thus the operator H is given as (Blokhintsev, 1964)

$$H = -\frac{\hbar^2}{2m} \sum_{i,k} \frac{1}{g} \frac{\partial}{\partial q_i} \left(g g^{ik} \frac{\partial}{\partial q_k} \right) \tag{3.1}$$

Substituting $p_{q_i}^\dagger$ as given by equation (2.5) into the Hamiltonian given by equation (2.4), we obtain

$$H = -\frac{\hbar^2}{2m} \sum_{i,k} \left(\frac{\partial}{\partial q_i} + \frac{1}{g}\frac{\partial g}{\partial q_i}\right) g^{ik} \frac{\partial}{\partial q_k}$$

$$= -\frac{\hbar^2}{2m} \sum_{i,k} \frac{\partial g^{ik}}{\partial q_i}\frac{\partial}{\partial q_k} + g^{ik}\frac{\partial^2}{\partial q_i \partial q_k} + \frac{1}{g}\frac{\partial g}{\partial q_i} g^{ik} \frac{\partial}{\partial q_k} \tag{3.2}$$

Thus H in equation (3.2) is identical to H given by equation (3.1) and we therefore obtain the correct representation of the Hamiltonian operator by our prescription of the momentum operator.

4. *Consequences*

In quantum theory, the generalized momentum operator 'squared', analogous to $p_{q_i}^* p_{q_i}$, is $p_{q_i}^\dagger p_{q_i}$, and is given as

$$`p_{q_i}^2\text{'} = p_{q_i}^\dagger p_{q_i} = -\hbar^2 \left(\frac{\partial}{\partial q_i} + \frac{1}{g}\frac{\partial g}{\partial q_i}\right)\frac{\partial}{\partial q_i} \tag{4.1}$$

Equation (4.1) may be rewritten as

$$`p_{q_i}^2\text{'} = p_{q_i}^\dagger p_{q_i} = -\hbar^2 \left(\frac{1}{g}\frac{\partial}{\partial q_i}\left(g\frac{\partial}{\partial q_i}\right)\right) \tag{4.2}$$

From equation (4.2), it is readily seen that in two dimensions ($g = r$) the correct form of the operator 'p_r^2' (that is, $p_r^* p_r$) in the corresponding Hamiltonian is given as

$$`p_r^2\text{'} = p_r^\dagger p_r = -\frac{\hbar^2}{r}\frac{\partial}{\partial r} r \frac{\partial}{\partial r}$$

Similarly, in three dimensions ($g = r^2 \sin\theta$) the correct operator form of the momenta 'p_r^2' and 'p_θ^2' in the corresponding three-dimensional Hamiltonian are given as respectively

$$`p_r^2\text{'} = p_r^\dagger p_r = -\frac{\hbar^2}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right)$$

$$`p_\theta^2\text{'} = p_\theta^\dagger p_\theta = -\frac{\hbar^2}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)$$

5. *Comments and Discussion*

We have shown in confirmation with the previous article (Gruber, 1971) that the correct operator form of the 'true' physical momentum in generalized coordinates is given as the Hermitian part of the operator $p_{q_i} = -i\hbar\,\partial/\partial q_i$. It is very interesting to note that classically, the product of generalized momentum operators, $p_{q_i} p_{q_k}$ in an observable quantity such as the Hamiltonian, is really to be represented as $p_{q_i}^* p_{q_k}$ whose quantum mechanical operator analog is the Hermitian part of the operator $p_{q_i}^\dagger p_{q_k}$, $(p_{q_i}^\dagger p_{q_k})^H$. Note that $(p_{q_i}^\dagger p_{q_k})^H = (p_{q_i}^\dagger p_{q_k} + p_{q_k}^\dagger p_{q_i})/2$. Here, $p_{q_i} = -i\hbar\,\partial/\partial q_i$. Thus the quantity '$p_{q_i}^2$' classically, if it is to have physical significance, is represented by $p_{q_i}^* p_{q_i}$ whose quantum mechanical operator analog is $(p_{q_i}^\dagger p_{q_i})^H = p_{q_i}^\dagger p_{q_i}$ where, as before, $p_{q_i} = -i\hbar\,\partial/\partial q_i$. The quantum mechanical operator analog for the momentum p_{q_i} (which classically could also be represented as $p_{q_i}^*$) is $(p_{q_i})^H = (-i\hbar\,\partial/\partial q_i)^H$ or if the momentum is classically represented as $p_{q_i}^*$, the quantum mechanical operator analog would be $(p_{q_i}^\dagger)^H$ which is shown to be equal to $(p_{q_i})^H$. Finally the generalized quantum mechanical Hamiltonian operator is written as

$$H = \frac{1}{2m} \sum_{i,k} p_{q_i}^\dagger g^{ik} p_{q_k}$$

where the generalized classical Hamiltonian is given as

$$H = \frac{1}{2m} \sum_{i,k} p_{q_i}^* g^{ik} p_{q_k}.$$

It is indeed interesting to see that the structure of the quantum mechanical Hamiltonian operator is based on products of $p_{q_i}^\dagger$ and p_{q_i} whereas the structure of the quantum mechanical 'observable' generalized momentum operator is based on a sum of the total momentum operator, $p_{q_i} = -i\hbar\,\partial/\partial q_i$ and its adjoint $p_{q_i}^\dagger$.

References

Blokhintsev, D. I. (1964). *Quantum Mechanics*, p. 517. D. Reidel Publishing Co., Dordrecht, Holland.

Brillouin, L. (1949). *Les Tenseurs en Mecanique et en Elasticite*, p. 200. Masson et Cie, Paris.

Gruber, G. R. (1971). *Foundations of Physics*, **1** (3), 227.

Pauli, W. (1950). *Die Allgemeinen Prinzipien der Wellenmechanik*, p. 120. J. W. Edwards Publishing Co., Ann Arbor, Michigan.

Sokolnikoff, I. S. (1951). *Tensor Analysis*. John Wiley & Sons, New York.