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Momentum and Hamiltonian Operators in Generalized Coordinates

Makoto Kato[1]

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The self-adjointness of momentum operators in generalized coordinates, questioned by Domingos and Caldeira is shown. The momentum operators of a particle and the kinetic part of its Hamiltonian operator constructed from them are characterized as self-adjoint operators and geometrical objects in coordinate-free form. Local coordinates of an n-dimensional Riemannian manifold are taken as the generalized coordinates of the particle. As an example the curvilinear coordinates of Euclidean space are treated. The coefficients of connection and curvature are given on the manifold for which the assumed momentum operators exist. It is found that if our momentum operators form a complete set of mutually commuting observables, the manifold is locally Euclidean, i.e., there exists a local coordinate system such that we obtain the usual Schrödinger correspondence rule.

1. INTRODUCTION

In quantum mechanics linear operators acting on wave functions correspond to physical quantities such as the coordinates and the momentum of particles and their functions, in terms of which classical mechanics is built up. These operators are expected to have the following properties:

(a) They satisfy Bohr's correspondence principle.

(b) The correspondence rule between classical quantities and these operators is invariant under coordinate transformations.

(c) They are self-adjoint.

(d) We arrive at the correct representation of the Hamiltonian operator of a free particle with mass m in the form

$$H = -\frac{1}{2m}\Delta \tag{1}$$

where Δ is the Laplace–Beltrami operator.

[1]Department of Physics, Tohoku Institute of Technology, Sendai, 982, Japan.

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Several authors have proposed various rules for producing quantum operators from classical quantities in generalized coordinates (e.g., see Gruber, 1971, and references therein). Properties (a) and (b) were studied in order to yield (d) mainly by Gruber (1971, 1972) and Castellani (1978), respectively. It seems to us that the operators do not satisfy some of the four properties (a–d) above. In particular, the question was raised by Domingos and Caldeira (1984) as to whether the momentum operators in generalized coordinates satisfy (c).

The purpose of this paper is to characterize the momentum operators and the kinematic part of the Hamiltonian operator of a particle in the coordinate representation as geometric objects of an n-dimensional Riemannian manifold independently of the coordinates chosen, so as to satisfy (b)–(d), taking the generalized coordinates of the particle as local coordinates of the manifold. They are defined as the differential operators corresponding to infinitesimal isometries with constant length which are mutually orthogonal at each point of the manifold and their homogeneous polynomial of degree 2 invariant under the isometries. In Section 2 we deal with the connection between the momentum operator and the group of translations (isometries) in the one-dimensional case. In Sections 3 and 4 we define the momentum operators and the Hamiltonian operator of a free particle by extending the considerations of Section 2 to the Riemannian manifold. It is shown that they satisfy (c) and (d). Property (a) is satisfied only for Cartesian coordinates of Euclidean space. Section 4 is devoted to the case of curvilinear coordinates of Euclidean space. In Section 5 we obtain the coefficients of connection and curvature of Riemannian manifolds for which there exist the momentum operators defined in Section 3.

2. MOMENTUM OPERATOR IN ONE DIMENSION

In the line $\mathbb{R}$ with coordinate x, we consider the group of translations $x = x + t$. The group of translation operators $T(t)$ acting on the set $L_2(-\infty, \infty)$ of all complex-valued functions of a real variable such that the square of their absolute values is integrable is defined by

$$(T(t)f)(x) = f(x+t), \qquad f \in L_2(-\infty, \infty)$$

Its infinitesimal generator A for differentiable functions in $L_2(-\infty, \infty)$ given by

$$(Af)(x) = \lim_{t \to 0} \frac{(T(t)f)(x) - f(x)}{t} = \lim_{t \to 0} \frac{f(x+t) - f(x)}{t} = \frac{df}{dx}(x)$$

regarded as an infinitesimal isometry which is a unit vector at each point x of $\mathbb{R}$.

Using the operator A, we define the momentum operator of a particle moving along $\mathbb{R}$ as $P = -iA$. The domain $D(P)$ of P is the set of all $f \in L_2(-\infty, \infty)$ for which df/dx exists and $df/dx \in L_2(-\infty, \infty)$. Since $D(P)$ is dense in $L_2(-\infty, \infty)$, there exists an operator adjoint to P. The operator P is self-adjoint (e.g., Akhiezer and Glazman, 1981) and the spectrum $\sigma(P)$ of P is the whole real axis $\mathbb{R}$. P possesses a complete system of eigenfunctions $e^{i\lambda x}$ belonging to the eigenvalues $\lambda \in \sigma(P)$. These eigenfunctions do not belong to $L_2(-\infty, \infty)$ and are considered as linear functionals on a test function space of infinitely differentiable functions of compact support.

We next consider the circle S' with coordinate θ and the group of translations on S^1. The infinitesimal generator of this group is expressed by $d/d\theta$, which is considered as an infinitesimal isometry with unit length. We regard $L = -i\, d/d\theta$ as the momentum operator of a particle in S^1. The domain $D(L)$ of L is the set of differentiable functions φ for which the boundary condition $\varphi(0) = \varphi(2\pi)$ is satisfied and $d\varphi/d\theta$ belongs to $L_2(0, 2\pi)$. L is self-adjoint operator in $L_2(0, 2\pi)$ (e.g., Akhiezer and Glazman, 1981). The eigenvalues of L are $m \in \mathbb{Z}$ and L possesses a complete system of eigenfunctions $e^{im\theta}$ belonging to $D(L)$.

3. FORMATION OF MOMENTUM OPERATORS IN A RIEMANNIAN MANIFOLD

In Euclidean space $\mathbb{R}$ the infinitesimal isometries consist of infinitesimal translations and rotations. The infinitesimal translations are represented by the vector fields $\partial/\partial x^i$ ($i = 1, 2, 3$) which are mutually orthogonal unit vectors at all points of $\mathbb{R}^3$ forming a basis of the Lie algebra of the translation group of $\mathbb{R}^3$, while the infinitesimal rotations cannot be represented by vector fields with constant length. Using the former vector fields, we can express the momentum operators P_i of a particle in $\mathbb{R}^3$ by

$$P = -i\frac{\partial}{\partial x^i}, \qquad i = 1, 2, 3$$

with the identification of differential operators on M. This fact leads us to the following definition of the momentum operators of a particle in a Riemannian manifold.

We consider the system of a particle and regard the generalized coordinates $q_1, q_2, \ldots, q_n$ of this particle as a local coordinate system $x = (x^1, x^2, \ldots, x^n)$ in a coordinate neighborhood U of an n-dimensional Riemannian manifold M with metric g. Corresponding to the group of translations of $\mathbb{R}^3$, we introduce a group G consisting of isometries of M and assume that there exists a set of infinitesimal isometries $X_1, X_2, \ldots, X_n$ of M which are n mutually orthogonal unit vectors with respect to g at each point of M and form a basis of a Lie algebra of vector fields on M isomorphic with the Lie algebra of the group G. If we take a local coordinate system $t = (t^1, t^2, \ldots, t^n)$ of G at the unit element of G and express the action of G on U of M as

$$x^{k'} = \phi^k(x, t), \qquad \phi^k \in C^\infty(U) \qquad (k = 1, 2, \ldots, n)$$

denoting the set of real analytic functions on U by $C^\infty(U)$, we can express the X_i in terms of these coordinate systems of M and G as

$$X_i = \xi^k_{(i)} \frac{\partial}{\partial x^k}, \qquad \xi^k_{(i)} \in C^\infty(U) \qquad (i = 1, 2, \ldots, n)$$

where we used the summation convention of repeated indices (this convention will be used throughout this paper) and put

$$\xi^k_{(i)} = \left[\frac{\partial \phi^k(x, t)}{\partial t^i}\right]_{t=0}$$

An orthogonal transformation of coordinate t

$$t^{j'} = a^j_i t^i$$

gives rise to a transformation of X_i such that

$$Y_j = a^i_j X_i, \qquad \text{where} \quad a^k_i a^k_j = \delta_{ij}$$

We define the momentum operators of the particle in M as

$$P_i = -iX_i \qquad \text{for each } i \tag{2}$$

identifying the vector fields with differential operators on M.

We denote the space of infinitely many times differentiable complex-valued functions with compact support in M by $C_0^\infty(M)$. For $f, h \in C_0^\infty(M)$ an inner product is defined by

$$(f, h) = \int_M f\bar{h}\, dv \tag{3}$$

where dv is the Riemannian measure of M. In terms of the local coordinate system in the neighborhood U of M, dv is expressed as

$$dv = [\det(g_{lm})]^{1/2}\, dx^1\, dx^2 \cdots dx^n, \qquad g_{lm} = g\left(\frac{\partial}{\partial x^l}, \frac{\partial}{\partial x^m}\right)$$

Using partition of unity, we interpret (3) as the integration over M.

Considering the P_i as the differential operators on $C_0^\infty(M)$, we express the formally adjoint operator P_i^* of P_i by

$$(P_i f, h) = (f, P_i^* h) \qquad \text{for all} \quad f, h \in C_0^\infty(M) \text{ and each } i$$

In terms of local coordinates of U, we have the expression

$$P_i^* f = iX_i^* f \tag{4}$$

for $f \in C_0^\infty(M)$ which has compact support inside U, where

$$X_i^* f = -\frac{1}{[\det(g_{lm})]^{1/2}} \frac{\partial}{\partial x^k} [\det(g_{lm})]^{1/2} \xi_{(i)}^k f = -X_i f - f \operatorname{div} X_i$$

Since X_i is the infinitesimal isometry, the components of X_i must satisfy Killing equations, from which we obtain

$$\operatorname{div} X_i = 0 \tag{5}$$

We denote a Hilbert space obtained by completion of $C_0^\infty(M)$ with respect to the inner product (3) by $L_2(M)$. Using the same notation as for the inner product on $C_0^\infty(M)$, we introduce the inner product on $L_2(M)$ by

$$(f, h) = \lim(f_n, h_n) \qquad \text{for } f, h \in L_2(M) \tag{6}$$

where $\{f_n\}$ is a Cauchy sequence in $C_0^\infty(M)$ corresponding to $f \in L_2(M)$. From the relations (4) and (5), we find that P_i is a symmetric operator, considered as a linear operator in $L_2(M)$.

We introduce the one-parameter subgroup $[\varphi_t : t \in \mathbb{R}\}$ of G generated by X_i for each X_i on M and define a family of linear operator $\{U(t): t \in \mathbb{R}\}$ by

$$U(t)f(p) = f(\varphi_t(p)) \qquad \text{for all} \quad f \in L_2(M) \quad \text{and} \quad p \in M \tag{7}$$

Since dv is invariant under the isometries of M, we have

$$(U(t)f, U(t)f) = (f, f), \qquad f \in C_0^\infty(M) \tag{8}$$

denoting the restriction of $U(t)$ to $C_0^\infty(M)$ by the same symbol. From (6), $U(t)$ defined by (7) satisfies the same relation as (8) for all $f \in L_2(M)$. As the result, it is a one-parameter group of unitary operators on $L_2(M)$. By Stone's theorem (e.g., Weidmann, 1980), the infinitesimal generator A_i of $U(t)$ is defined in $L_2(M)$ and $-iA_i$ is self-adjoint, which is the self-adjoint extension of P_i as a linear operator in $L_2(M)$.

4. CONSTRUCTION OF THE HAMILTONIAN OPERATOR FROM THE MOMENTUM OPERATORS

The classical Hamiltonian of a particle moving freely in M is considered to be

$$H_c = \frac{1}{2m} g^{ij} p_i p_j$$

where (g^{ij}) is the inverse of (g_{ij}) and p_k is the canonical momentum of the particle conjugate to x^k. Since the inverse of $(g(X_i, X_j)) = (\delta_{ij})$ is (δ^{ij}), using the momentum operators defined by (2), we define the quantum Hamiltonian operator of the particle in M corresponding to H_c by the linear operator

$$H = \frac{1}{2m}\delta^{ij}P_iP_j = -\frac{1}{2m}\delta^{ij}X_iX_j \tag{9}$$

acting on the subset of the space $L_2(M)$. From (4) and (5) we have

$$(P_iP_j)^* = P_j^*P_i^* = P_jP_i$$

We find that H defined by (9) is formally self-adjoint and symmetric in $L_2(M)$. Since H is real, it has self-adjoint extensions (e.g., Weidmann, 1980). From our assumption for X_i and (5) it follows that

$$\Delta f = \operatorname{div}\operatorname{grad} f = \operatorname{div}((X_if)X_i) = \delta^{ij}X_iX_j$$

from which we know that (9) becomes (1).

5. CURVILINEAR COORDINATES

We take curvilinear coordinates u^i $(i = 1, 2, 3)$ in the space $\mathbb{R}^3$ with the natural coordinates x^i $(i = 1, 2, 3)$. In this case the components of g and g^{-1} are given by

$$g_{ij} = \frac{\partial x^k}{\partial u^i}\frac{\partial x^k}{\partial u^j}, \qquad g^{ij} = \frac{\partial u^i}{\partial x^k}\frac{\partial u^j}{\partial x^k}$$

For example, the vector fields

$$X_i = \frac{\partial u^k}{\partial x^i}\frac{\partial}{\partial u^k}$$

are the infinitesimal isometries which are orthonormal with respect to g at each point of the domain in $\mathbb{R}^3$ that u^i are regarded as a local coordinate system, because they satisfy

$$g_{kl}\frac{\partial u^k}{\partial x^i}\frac{\partial u^l}{\partial x^j} = \delta_{ij}$$

and Killing's equations. According to (2), in this choice of the basis of the Lie algebra of the infinitesimal isometries of $\mathbb{R}^3$, the momentum operators are given by

$$P_i = -iX_i = i\frac{\partial u^k}{\partial x^i}\frac{\partial}{\partial u^k}$$

They are different from the Schrödinger prescription $-i\,\partial/\partial u^i$, which are not always self-adjoint.

As an example, we take spherical coordinates (r, θ, φ) in $\mathbb{R}^3$ with the x^3 axis removed, we have

$$X_1 = \sin\theta\cos\varphi\frac{\partial}{\partial r} + \frac{\cos\theta\cos\varphi}{r}\frac{\partial}{\partial\theta} - \frac{\sin\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}$$

$$X_2 = \sin\theta\sin\varphi\frac{\partial}{\partial r} + \frac{\cos\theta\sin\varphi}{r}\frac{\partial}{\partial\theta} + \frac{\cos\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}$$

$$X_3 = \cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial\theta}$$

6. ASSUMED RIEMANNIAN MANIFOLDS

We consider the Riemannian manifolds which satisfy the conditions assumed in Section 3. The orthonormal basis $\{X_i\}$ of the infinitesimal isometries identified with the basis of the Lie algebra of G satisfies

$$[X_i, X_j] = c_{ij}^k X_k$$

where c_{ij}^k are the structure constants of the Lie algebra with respect to the basis. From the conditions assumed for the manifold, we find that c_{ij}^k are completely skew symmetric. In terms of these structure constants, the coefficients of the Riemannian connection and curvature of M with respect to the basis are given by

$$\Gamma_{ij}^k = \tfrac{1}{2}c_{ij}^k, \qquad R_{kij}^l = -\tfrac{1}{4}c_{ij}^m c_{mk}^l$$

If our momentum operators form a complete set of commuting observables, we find that M is locally Euclidean; then there is a local coordinate system such that we have the Schrödinger rule for the momentum operators. In particular, for a particle in a two-dimensional manifold, all the structure constants are zero, so that there exists no momentum operators defined by us unless the manifold is locally Euclidean. In order to define the momentum operators for such manifolds, we weaken the definition of momentum operators in the following form. We assume that there exist n linearly independent vector fields $X_1, X_2, \ldots, X_n$ everywhere on M satisfying (5); then we define the momentum operators of a particle in M by (2). The Hamiltonian operator constructed from them is given in place of (9) by

$$H = \frac{1}{2m}P_i h^{ij} P_j$$

where (h^{ij}) is the inverse of $(h_{ij}) = (g(X_i, X_j))$.

7. CONCLUSIONS

We have defined the momentum operators in M by (2). Using them, we have constructed the Hamiltonian operator of the free particle by (5). These momentum operators are not necessarily commutative and the commutation relations between them and H are given by

$$[P_i, P_j] = i d_{ij}^k P_k, \qquad [H, P_l] = 0$$

where d_{ij}^k are skew-symmetric real constants. If they form a set of mutually commuting observables, M is locally Euclidean and there exists a local coordinate system in M for which we obtain the usual Schrödinger correspondence rule.

In the case of curvilinear coordinates of $\mathbb{R}^3$, our definitions contain the usual procedure: When applying the correspondence rule with Schrödinger's prescription, the coordinates and momenta must be expressed in Cartesian coordinates and then one goes over to curvilinear coordinates by carrying out a change of variables. Our method has given this procedure a geometrical meaning. The momentum and the Hamiltonian operators thus defined satisfy (b), (c), and (d). Property (a) is not satisfied except for Cartesian coordinates of $\mathbb{R}^3$. The physical quantities of the classical mechanical system represented by the variables q_i and p_i are also described by q_i' and p_i', which are the canonical transformation of q_i and p_i. Corresponding to all these classical quantities, it seems difficult to construct the quantum mechanical counterparts which satisfy all the properties (a)–(d), because of different algebras and transformations.

As a result of the momentum and the Hamiltonian operators satisfying (c), if for a self-adjoint operator A, any one of the momentum and the Hamiltonian operators, we can choose a nuclear space D containing $C_0^\infty(M)$ such that D is dense in $L_2(M)$ and A maps D into itself, we have the inclusions: $D \subset L_2(M) \subset D'$, where D' is the dual space of D, and find that A possesses a complete system of eigenfunctionals belonging to D' by the theorem of self-adjoint operators (Gel'fand and Shilov, 1976).

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