Geometric momentum for a particle constrained on a curved hypersurface

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The canonical quantization is a procedure for quantizing a classical theory while preserving the formal algebraic structure among observables in the classical theory to the extent possible. For a system without constraint, we have the so-called fundamental commutation relations (CRs) among positions and momenta, whose algebraic relations are the same as those given by the Poisson brackets in classical mechanics. For the constrained motion on a curved hypersurface, we need more fundamental CRs otherwise neither momentum nor kinetic energy can be properly quantized, and we propose an enlarged canonical quantization scheme with introduction of the second category of fundamental CRs between Hamiltonian and positions, and those between Hamiltonian and momenta, whereas the original ones are categorized into the first. As an \( N - 1 \) \((N \geq 2)\) dimensional hypersurface is embedded in an \( N \) dimensional Euclidean space, we obtain the proper momentum that depends on the mean curvature. For the spherical surface, a long-standing problem in the form of the geometric potential is resolved in a lucid and unambiguous manner, which turns out to be identical to that given by the so-called confining potential technique. In addition, a new dynamical group \( SO(N, 1) \) symmetry for the motion on the sphere is demonstrated.

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I. INTRODUCTION

The quantum mechanics for a non-relativistic particle that is constrained to remain on a curved hypersurface attracts much attention. As well-known, the current understanding of the Dirac’s canonical quantization procedure for a constrained motion does not always produce physically significant results and usually exhibits certain difficulties in application, from which we do not even know an unambiguous form of momentum or Hamiltonian after quantization. A fundamental yet controversial issue is that the canonical quantization entails using Cartesian coordinates, but the Cartesian coordinates exist only in flat spaces.

In this paper, we present an enlarged canonical quantization (ECQ) scheme for the constrained motion on the hypersurface based on the Dirac’s canonical quantization, and then explicitly deal with an \( N - 1 \) \((N \geq 2)\) dimensional one \( S^{N-1} \) whose equation takes either form \( f(\mathbf{x}) = 0 \) or a parametric one \( \mathbf{x} = \{x_i(u)\} \) in the \( N \) dimensional flat ambient space \( R^N \), where \( x_i \) \((i, j, k, \ell = 1, 2, 3, \ldots, N)\) stand for the Cartesian coordinates and \( u^\mu \) \((\mu, \nu = 1, 2, 3, \ldots, N - 1)\) symbolize the local coordinates on the surface. According to Dirac, such a hypersurface belongs to the second-class constraint. In our approach, we do not quantize the local coordinates \( u^\mu \) or corresponding momenta \( p_\mu \) but treat \( u^\mu \) as parameters, and we quantize the Cartesian coordinates \( x_i \) and their corresponding momenta \( p_i \).

For a particle constrained on the hypersurface, we have an effective theory in the following way. First, to formulate the Schrödinger equation in \( R^N \), explicitly in a curved shell of an equal and finite thickness \( \delta \) along normal direction \( \mathbf{n} \), and let the intermediate surface of the shell coincide with the prescribed one \( S^{N-1} \). Thus, the particle moves within the range of the same width \( \delta \) due...
to a confining potential, such as one-dimensional parabolic one or simply the square potential well, across the surface along the normal direction \( \mathbf{n} \). Second, to take the limit \( \delta \to 0 \), we have an effective kinetic energy operator that differs from the well-known one \( -\hbar^2/(2m)\nabla_L^2 \), and is given by

\[
-\frac{\hbar^2}{2m} \nabla_L^2 \rightarrow -\frac{\hbar^2}{2m} (\nabla_L^2 + v_g) , \quad v_g = \frac{1}{4} (2Tr(k)^2 - (Tr(k^2)) ,
\]

where \( V_g \equiv -\hbar^2/(2m)v_g \) is the curvature-induced potential that is usually called the geometric potential, and \( v_g \) is purely determined by the principal curvatures \( k \). We thus obtain an effective Schrödinger equation for the particle constrained on the surface.

This effective approach is straightforward and physically reasonable, but raises a question: Can we build a quantum theory directly on the surface \( S^{N-1} \) without considering the underlying flat ambient space? In other words, can the canonical quantization be accomplished within the intrinsic geometry? We recently examine such a question with a proposed ECQ scheme for a particle on the \( S^2 \), and show that the answer is in general negative for there are many counterexamples. The present paper explores further problems: the ECQ for the particle on the \( S^{N-1} \) and its main consequences. Since the geometric potential must be dealt with on the case-by-case basis, we treat the motion on the \( N-1 \) dimensional spherical surface, and successfully resolve a long-standing and highly controversial problem as to how the canonical quantization reproduces the same geometric potential as predicted by Eq. (1). Moreover, the general and compact form of the geometric momentum for the motion on an arbitrary curved hypersurface is obtained.

The organization of the paper is as follows. In Sec. II, the full form of the ECQ is given, and as a consequence the geometric momentum is given in Sec. III. In Sec. IV, by use of the ECQ we deal with the geometric potential for a particle on an \( N-1 \) dimensional spherical surface and thus resolve a long-standing and highly controversial problem on the form of the geometric potential. In Sec. IV, we show that the motion on the surface possesses a dynamical \( SO(N, 1) \) group symmetry. In Sec. V, we conclude and remark the present approach. This paper contains a short appendix that collects two relations for hypersurfaces which are useful for our derivations of results. The Einstein summation convention for repeated indices is used throughout the paper, and only the free motion on the hypersurface is considered without loss of generality.

## II. SECOND CATEGORY OF FUNDAMENTAL COMMUTATION RELATIONS AND ECQ

The canonical quantization is a procedure for quantizing a classical theory while preserving the formal algebraic structure among observables in the classical theory to the extent possible. For simple systems without constraint such as hydrogen atom and simple harmonic oscillator, only the algebraic relations among positions and momenta matter. As a consequence, the equation of motion \( dO/dt = [O, H]_P \) for an observable \( O \) remains the same form as that in quantum theory \( dO/dt = (i\hbar)[H, O]_{\mathcal{D}} \), where \( [O_1, O_2]_P \) denotes the Poisson bracket. This is why we have the fundamental commutation relations (CRs) in which only nontrivial ones are \( [x_i, p_j] = i\hbar \delta_{ij} \) and all other commutators vanishing. This is the fundamental postulate for positions and momenta in quantum mechanics, proposed by Dirac, without requiring them to be Cartesian. It holds true universally if applicable, but is not so practical for, e.g., a system that does have a classical analogue. Dirac noted it and immediately developed his fundamental CRs with an additional hypothesis that the Hamiltonian would not be the same function of the canonical coordinates and momenta in the quantum theory as in the classical theory, unless the Cartesian coordinates are used. This is why many, including us, take for granted that the Cartesian coordinates in the underlying flat Euclidean space must be used in performing the canonical quantization, and the existence of the flat space is considered a fundamental postulate in non-relativistic quantum mechanics. It is also understandable that not everyone shares this point of view so various schemes of quantization develop.

For a system with constraints of the second-class, the fundamental CRs in the Dirac’s canonical quantization procedure must be enlarged because the classical-quantum correspondence \( [O_1, O_2] \equiv i\hbar [O_1, O_2]_{\mathcal{D}} \) for two observables \( O_1, O_2 \) does no longer hold true automatically, where \( [O_1, O_2]_D \) denotes the Dirac bracket. In fact, from the known fundamental CRs, there are many forms of the momentum \( \mathbf{p} \), and with substituting these forms of \( \mathbf{p} \) into
Hamiltonian such as $H = p^2/2m + V$, there are various forms of Hamiltonian in quantum mechanics. The proper forms of the momentum and the Hamiltonian cannot be determined unless more CRs between observables \([O_1, O_2]_D\) in classical mechanics are imposed as fundamental ones as \([O_1, O_2] \equiv \hbar [O_1, O_2]_D\) while quantizing the classical theory. Fundamentally, we introduce the second category of fundamental CRs as \([x, H] \equiv i\hbar [x, H]_D\) and \([p, H] \equiv i\hbar [p, H]_D\), while the existent ones are classified into the first, which are for positions and momenta \((x, p)\). This is the so-called ECQ.

An observation concerning the ECQ follows. For an intrinsic description of a hypersurface, the global Cartesian coordinate system does not exist and even the local one \(\{u^\mu\}\) can be used approximately. Because the local coordinates \(\{u^\mu\}\) must never be Cartesian, the second category of fundamental CRs \([u^\mu, H] \equiv (i\hbar)[u^\mu, H]_D\) and \([p_\mu, H] \equiv (i\hbar)[p_\mu, H]_D\) would hardly be all satisfied, as stressed by Dirac\(^{17}\) and other authors\(^{21–23}\) and illustrated in Refs.\(^{12–14}\). So, the fundamental importance of the Cartesian coordinates within the canonical quantization procedure excludes the possibility of an attempt to get the proper form of the quantum Hamiltonian by means of a direct quantization of the local coordinates \(\{u^\mu\}\) and their generalized momentum \(\{p_\mu\}\).\(^{17,21–23}\) As a consequence of this observation, we resort to \(R^N\) to deal with \(S^{N–1}\) that is embedded in \(R^N\) to perform the canonical quantization.

For the \(N–1\) dimensional surface, we conveniently choose the surface \(f(x) = 0\) such that \(\nabla f(x) = 1\) so \(n \equiv \nabla f(x)\) being the normal at a local point \(\{u^\mu\}\), and \(g_{\mu\nu} \equiv \partial x/\partial u^\mu \cdot \partial x/\partial u^\nu\). \(\partial x/\partial u^\nu = x_\mu \cdot x_\nu\) where \(O_{\mu\nu} \equiv \partial O/\partial u^\mu \cdot \partial O/\partial u^\nu\) and \(O_{\mu\nu} = g_{\mu\nu} O_{\nu\sigma} \). For a particle constrained on the surface, we have a compatible constrained condition\(^{1,6,27,28}\)

\[
\mathbf{n} \cdot \mathbf{p} = 0. \tag{2}
\]

The first category of fundamental CRs is\(^{1,6,27,28}\)

\[
[x_i, x_j] = 0, \quad [x_i, p_j] = \imath \hbar (\delta_{ij} - n_in_j), \quad [p_i, p_j] = -\imath \hbar \left\{n_in_k,j - n_jn_k,i\right\}_{\text{Hermitian}},
\]

where \(O_{\text{Hermitian}}\) stands for a suitable construction of the Hermitian operator of an observable \(O\). Because the free particle Hamiltonian in classical mechanics takes the form \(H = p^2/2m\), we have\(^{6}\) \([x, H]_D = p/m\), and \([p, H]_D = -n_in_j p_j p_k\). The second category of fundamental CRs is then given by

\[
\mathbf{p} = \frac{i}{\hbar} [H, \mathbf{x}], \quad [H, \mathbf{p}] = \frac{i\hbar}{m} (\mathbf{n}p_k p_j)_{\text{Hermitian}}. \tag{4}
\]

Once curved surface \(f(x) = 0\) becomes flat, both the momentum and the Hamiltonian must assume their usual forms, respectively. Thus, we make an ansatz for the quantum \(H\) to take the following form with a potential \(V_g\) which must be a geometric invariant:

\[
H = -\hbar^2/(2m)\nabla_{LB}^2 + V_g. \tag{5}
\]

### III. GEOMETRIC MOMENTUM

First of all, we have the momenta \(\mathbf{p}\) from Eqs. (4) and (5),

\[
\mathbf{p} = \frac{i}{\hbar} \left[\nabla_{LB}^2, \mathbf{x}\right] = -\frac{\hbar}{2} \left(\left(\nabla_{LB}^2 \mathbf{x}\right) + 2\mathbf{x}^\mu \delta_{\mu}\right) = -\imath \hbar (\nabla_S + \frac{M\mathbf{n}}{2}), \tag{6}
\]

where a relation \(\nabla_{LB}^2 \mathbf{x} = M\mathbf{n}\) is used (cf. Appendix). We call \(\mathbf{p}\) \((\ref{6})\) the geometric momentum for its dependence on the extrinsic curvature \(M\).\(^{41–44}\)

Second, we demonstrate that the operator version of the constrained condition (2) for the momenta \(\mathbf{p}\):

\[
\mathbf{p} \cdot \mathbf{n} + \mathbf{n} \cdot \mathbf{p} = 0. \tag{7}
\]

It is evident for the action of the vector operator \(\nabla_S\) on the unit normal vector \(\mathbf{n}\) leads to a nonvanishing result as \(\nabla_S \cdot \mathbf{n} = -M\) (cf. Appendix), which exactly cancels \(M\) in \((\nabla_S + M\mathbf{n}/2) \cdot \mathbf{n} + \mathbf{n} \cdot (\nabla_S + M\mathbf{n}/2) = 0\) so that we have the quantum mechanical version of the orthogonal relation (7).
Finally, we need to show that the first category of the fundamental CRs is satisfied with this momenta \( p \) (6). A verification of the first two fundamental CRs in (3) is straightforward. The proof of the last in (3) is also an easy task. The key step is a proper construction of the Hermitian operator of observable \( O \). Only the following naive rule \((O + O')/2\) is used:

\[
\{n_i n_{k,j} p_k\}_\text{Hermitian} = \frac{1}{2} (n_i n_{k,j} p_k + p_k n_i n_{k,j}) = n_i n_{k,j} p_k + \frac{1}{2} (-i\hbar) (n_i\delta_{k,j} + n_j\delta_{i,k} + n_i\partial_j M).
\]

It is applicable in the RHS of the fundamental CRs \([p_i, p_j] = -i\hbar\{n_i n_{k,j} - n_j n_{k,i}\}p_k\)_\text{Hermitian} as

\[
\{(n_i n_{k,j} - n_j n_{k,i}) p_k\}_\text{Hermitian} = \{n_i n_{k,j} p_k\}_\text{Hermitian} - (i \leftrightarrow j).
\]

For a two-dimensional spherical surface, how to measure the geometric momenta (6) in molecular systems is extensively investigated. 28, 30

### IV. GEOMETRIC POTENTIAL FOR QUANTUM MOTION ON SPHERICAL SURFACE

With the first category of the fundamental CRs being used only, we have at least ten choices of \( \alpha(N) \) in \( V_g = \alpha(N)\hbar^2/(2mr^2) \), based upon various understanding of the problem. For instance, on the dependence of \( V_g \) on the dimensions \( N \), we have, (1) \( \alpha(N) = 0 \), (2) \( \alpha(N) = (N - 1)^2/4, 28 \) (3) \( \alpha(N) = (1 + 4s^2)(N - 1)^2/4 \) with \( s \) being a real parameter, (4) \( \alpha(N) = N^2/4, 35 \) (5) \( \alpha(N) = (N - 1)(N + 1)^2/4, 28 \) (6) \( \alpha(N) = (N - 1)N/4 \), (7) \( \alpha(N) = (N - 3)(N + 1)/4 \), (8) \( \alpha(N) = (N - 1)(N - 2)\beta, 28 \) (9) \( \alpha(N) \) arbitrary, 31 and (10) \( \alpha(N) = (N - 1)(N - 3)/4 \). At first sight, these disputant results seem to be rather irrelevant. Common experiments are only capable of detecting energy differences, in which these constants drop out. Cosmology, however, is sensitive to an additive constant. 1, 31

Now let us see what \( V_g \) is within our ECQ. The first category of the fundamental CRs is 28, 31

\[
[x_i, x_j] = 0, [x_i, p_j] = i\hbar(\delta_{ij} - n_i n_j), \{p_i, p_j\} = -i\hbar(x_i p_j - x_j p_i)/r^2.
\]

No operator ordering problem occurs in the RHS of \([p_i, p_j]\) because of the Jacobi identity. We see already that these relations (10) are automatically satisfied with Cartesian coordinates \( x \) and geometric momentum \( p \) (6). Now we examine the remaining fundamental CRs in the second category (4) which is given by, with noting relations \( n = x/r \) and \( n_i, j = (\delta_{ij} - n_i n_j)/r \) so \( p_i, p_j = p_i r = 2mH/r \). \( H = x^2 + Hx \),

\[
[H, p] = i\hbar \frac{xH + Hx}{r^2}.
\]

On the one hand, because the geometric potential \( V_g \) results from the noncommutability of different components of the geometric momentum (6), it depends solely on the geometric invariants as the geometric momentum does. On the other hand, all principal curvatures for the spherical surface are the same \(-1/r\) and the mean curvature is \( M = -(N - 1)/r \). So, the geometric potential \( V_g \) also takes the form \( \alpha(N)\hbar^2/(2mr^2) \) and the Hamiltonian takes the form \( H = -\hbar^2/(2m)\nabla_{LB}^2 + \alpha(N)\hbar^2/(2mr^2) \).

We will prove

\[
V_g = \frac{(N - 1)(N - 3)}{4} \frac{\hbar^2}{2mr^2},
\]

which is exactly the geometric potential \( V_g \) for the surface under consideration. The proof is as what follows.

The Hamiltonian \( H \) can be rewritten in the following form:

\[
H = -\frac{\hbar^2}{2m} \nabla_{LB}^2 + V_g = \frac{p^2}{2m} - M^2\hbar^2 \frac{h^2}{8m} + V_g,
\]

and so the quantity \( (xH + Hx) \) becomes

\[
xH + Hx = 2xH - i \frac{\hbar}{m} p.
\]
The RHS of the fundamental CRs (11) is
\[
\frac{i\hbar}{r^2} x H + H x = \frac{i\hbar}{mr} \left( np^2 - \frac{M^2\hbar^2}{4} + 2nmV_g - \frac{i\hbar}{r} p \right). 
\] (15)

The LHS of (11) \([H, p] = [p^2, p]/(2m)\) is, with repeated use of the first category of fundamental CRs (10),
\[
\frac{1}{2m}[p^2, p] = \frac{i\hbar}{mr} \left( np^2 + \frac{\hbar^2}{2r} nM - \frac{i\hbar}{r} p \right). 
\] (16)

Multiplying the results (15) and (16) by the unit normal vector \(n\) from the left, we obtain (12).

\[Q.E.D.\]

It is interesting to point out that the geometric momenta \(p\) and the angular momenta \(L_{ij} \equiv x_i p_j - x_j p_i\) form a closed \(so(N, 1)\) algebra. Let \(P_t \equiv r p_t\), we have from (10)
\[
[P_t, P_j] = -i\hbar L_{ij}. 
\] (17)

It is easy to show that the components of the angular momentum satisfy the standard \(so(N)\) algebra from its definition of \(L_{ij}\) and fundamental CRs (10),
\[
[L_{ij}, L_{k\ell}] = -i\hbar \left(-\delta_{i\ell} L_{kj} + \delta_{ik} L_{\ell j} + \delta_{jk} L_{i\ell} - \delta_{j\ell} L_{ik} \right). 
\] (18)

The commutation relation between \(L_{ij}\) and \(P_t\) is, with also repeated use of the first category of fundamental CRs (10),
\[
[L_{ij}, P_t] = i\hbar \left( \delta_{i\ell} P_j - \delta_{j\ell} P_i \right). 
\] (19)

These generators \(L_{ij}\) and \(P_t\) form a closed \(so(N, 1)\) algebra, which reflects a dynamical \(SO(N, 1)\) group symmetry beyond its geometrical one \(SO(N)\). It implies that there is a dynamical representation that can be used to examine the motion on the spherical surface.

V. CONCLUSIONS AND REMARKS

The usual canonical quantization procedure contains only the first category of the fundamental CRs, forming the invariable part of the procedure, therefore universally valid. For a particle constrained to remain on a curved hypersurface, the different components of momentum are not mutually commutable. Thus, the procedure of obtaining the quantum Hamiltonian by a simple substitution of an expression of the momentum into the Hamiltonian \(H = p^2/2m\) has been an issue full of debates, and is therefore questionable. A further strengthening of the quantization procedure is needed, and we propose to use the second category of the fundamental CRs to determine the forms of both the quantum momentum and Hamiltonian. The present study shows that there is a universal form of the momentum, the geometric momentum, and there is a concise and lucid way to produce the geometric potential for the spherical surface. Moreover, we demonstrate that there is a dynamical \(SO(N, 1)\) group symmetry on the surface beyond the geometrical one \(SO(N)\).

There are interesting issues which will be explored in near future: the relation between the geometric momentum and annihilation operators on the \(N - 1\) dimensional sphere, and a possibly universal form of a construction of the operator \(\left( n_k, j p_k, p_j \right)_{\text{Hermition}} \) rather than a treatment on the case-by-case basis, and the possible influence of the geometric potential on the dark energy as a consequence of embedding our universe in higher dimensional flat space-time, etc.

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APPENDIX: TWO DIFFERENTIAL GEOMETRIC RELATIONS FOR HYPERSONSURFACES

(1) The definition of the mean curvature \( M = Tr k = - \partial n_j / \partial x_j \) (rather than a true average \( T r k/(N-1) \) which is also widely used), and the mean curvature vector \( \mathbf{M} \) which satisfies \( \nabla_k \mathbf{n} = - \mathbf{M} \), where the surface gradient \( \nabla_n \) is defined by the difference of the usual gradient \( \nabla \mathbf{v} \) in \( \mathbb{R}^N \) and its component along the normal direction \( \mathbf{n} \partial_n \), \( \nabla_k \equiv (\partial \mathbf{x} / \partial u^i) \partial^i \equiv \mathbf{e}_i (\delta_{ij} - n_i n_j) \partial_j = \nabla_N - \mathbf{n} \partial_n \), with \( \mathbf{e}_i \) being the unit vector of the \( i \)th Cartesian coordinate and \( \delta_{ij} - n_in_j \) being the orthogonal projection from \( \mathbb{R}^N \) to the plane tangential to the \( S^{N-1} \).

(2) The Laplace-Beltrami operator \( \nabla^2 \) is given by \( \nabla^2 M = \nabla_N \mathbf{S} \) with \( \nabla_N \equiv \partial / \partial t \), the usual Laplacian operator, and \( \mathbf{S} = \mathbf{M} \). It is evident that \( \nabla^2 M, \nabla_N \mathbf{S}, \) and \( \mathbf{M} \) are all geometric invariants.