Identification of Geometric Potential from Quantum Conditions for a Particle on a Curved Surface

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Combination of a construction of unambiguous quantum conditions out of the conventional one and a simultaneous quantization of the positions, momenta, angular momenta and Hamiltonian leads to the geometric potential given by the so-called thin-layer quantization.

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I. INTRODUCTION

In quantum mechanics for a system, the construction of a proper quantum Hamiltonian operator takes the central position. For a free particle constrained to live on a curved surface or a curved space, DeWitt in 1957 used a specific generalization of Feynman’s time-sliced formula in Cartesian coordinates and found a surprising result that his amplitude turned out to satisfy a Schrödinger equation different from what had previously assumed by Schrödinger and Podolsky. In addition to the kinetic term which is Laplace-Beltrami operator divided by two times of mass, his Hamilton operator contained an extra effective potential proportional to the intrinsic curvature scalar.

[2] and Podolsky [3]. In addition to the kinetic term which is Laplace-Beltrami operator divided by two times of mass, the effect term which is Laplace-Beltrami operator divided by two times of mass, his Hamilton operator contained an extra effective potential proportional to the intrinsic curvature scalar.

Jensen and Koppe in 1972 [4] and subsequently da Costa [5] in 1981 developed a thin-layer quantization (also known as confining potential formalism) to deal with the free motion on the curved surface and demonstrated that the particle experiences a quantum potential that is a function of the intrinsic and extrinsic curvatures of the curved surface, which was later called the geometric potential [6]. By the thin-layer quantization we mean a treatment of \( (n-1) \)-dimensional smooth surface \( S^{n-1} \) in flat space \( R^n \) \((n \geq 1) \) and two infinitely high potential walls at the distance \( \delta \to 0 \) from the surface. Since the excitation energies of the particle in the direction normal to the surface are much larger than those in the tangential direction so that the degree of freedom along the normal direction is actually frozen to the ground state, an effective dynamics for the constrained system on the surface is thus established. This thin-layer quantization has a distinct feature for no presence of operator-ordering difficulty or other ambiguities. It is thus a powerful tool to examine various curvature-induced consequences in low-dimensional curved nanostructures, for instance, spin-orbit interaction of electrons on a curved surface [7], the mechanical-quantum-bit states [8], the geometry-induced charge separation on helicoidal ribbon [9], the curvature-induced p-n junctions in bilayer graphene [10], the periodic curvature dependent electrical resistivity of corrugated semiconductor films [11] as well as the geometry-driven shift in the Tomonaga-Luttinger liquid [12], electronic band-gap opening in corrugated graphene [13], low-temperature resistivity anomalies in periodic curved surfaces [14], curvature effects in thin magnetic shells [15], and the induced magnetic moment for a spinless charged particle on a curved wire [16], etc. [16–20] Experimental confirmations include: an optical realization of the geometric potential [21] in 2010 and the geometric potential in a one-dimensional metallic \( C_{60} \) polymer with an uneven periodic peanut-shaped structure in 2012 [22]. Applying the thin-layer quantization to momentum operators which are fundamentally defined as generators of a space translation, we have geometric momenta [23] which depends on the extrinsic curvatures of the curved surface.

It is generally accepted that the canonical quantization offers a fundamental framework to directly construct the quantum operators, and the fundamental quantum conditions are commutators between components of position and momentum [24, 25]. Many explorations have been devoted to searching for the geometric potential within the framework [26, 27]. It is curious that no attempt is successful for even simplest two-dimensional curved surface \( S^2 \) embedded in \( R^3 \). The best result was to start from surface equation \( df(x)/dt = 0 \), the time \( t \) derivative of the direct one \( f(x) = 0 \) rather than \( f(x) = 0 \) itself, to obtain a potential depending on the the intrinsic and extrinsic curvatures via two arbitrary real coefficients [30]. Some results are contradictory with each other, for instance, for a free particle on a \( (n-1) \)-dimensional sphere Kleinert and Shabanov predicted no existence of any quantum potential [31], whereas the thin-layer quantization presented \((n-1)(n-3)\) for such a multiple [28]. We revisited all these attempts, and concluded that the canonical quantization together with Schrödinger-Podolsky-DeWitt approach of Hamiltonian operator construction was dubious, for the kinetic energy in it takes some presumed forms that are primarily a sum of the Cartesian momenta squared. Since 2011, we have tried to enlarge the canonical quantization scheme to simultaneously quantize the Hamiltonian together with positions and momenta [10], rather than substituted the position and momentum operators into some presumed forms of Hamiltonian. Yet the success is limited. i) We obtained the geometric momentum which
In classical mechanics, the Hamiltonian is simply the Hamiltonian together with the fundamental quantities as position, momentum and the Hamiltonian includes correct form of the geometric potential. It is the first time to achieve this result within the angular momentum, the Hamiltonian includes correct form of the geometric potential. It is the first time to achieve this result within the classical mechanics, the Hamiltonian is simply $H = p^2/2\mu$ where $p$ denotes the momentum, and $\mu$ denotes the mass. However, in quantum mechanics, we cannot impose the usual canonical commutation relations $[x_i, p_j] = \pmih\delta_{ij}$, $(i, j = 1, 2, 3)$. Dirac was aware of the fact the presence of this constraint which needed to be eliminated before quantization could very well cause the remaining classical phase to not admit Cartesian coordinates.

In this Letter, we report that for a particle on a two-dimensional curved surface, simultaneous quantization of the constraint matrix $(C_{\alpha\beta})$ and the functions $\chi_{\alpha}(q, p)$ $(\alpha, \beta = 1, 2)$ are two constraints [38],

$$\chi_1(x, p) \equiv f(x) (= 0), \text{ and } \chi_2(x, p) \equiv n \cdot p (= 0).$$

The bracket $[f(x, p), g(x, p)]_D$ is called the Dirac bracket. We have elementary Dirac brackets in the following, with use of symbol $n_{ij} \equiv \partial n_i/\partial x_j$ [38],

$$[x_i, x_j]_D = 0, \quad [x_i, p_j]_D = \delta_{ij} - n_i n_j, \quad [p_i, p_j]_D = (n_j n_{i,k} - n_i n_{j,k})p_k. \quad (3-5)$$

These brackets were in general taken the fundamental set which after quantization forms the set of the so-called fundamental quantum conditions [24, 25]. In classical mechanics, the motion particle follows the geodesic whose surface. We do not use the conventional symbol $L$ that is usually used to denote the orbital angular momentum where the orbital angular momentum.

Next, we have following equations of motion for $x, p$ and $G$, respectively,

$$\frac{dx}{dt} \equiv [x, H]_D = \frac{p}{\mu}, \quad (7)$$
$$\frac{dp}{dt} \equiv [p, H]_D = -\frac{n}{\mu}(p \cdot \nabla n \cdot p), \quad (8)$$
$$\frac{dG}{dt} \equiv [G, H]_D = - (x \cdot n) \frac{p \cdot \nabla n \cdot p}{\mu} = T. \quad (9)$$

Dirac gave a general theory for a large class of constrained Hamiltonian systems including the motion on the surface $[24]$. He introduced a bracket instead of the Poisson one $[f(x, p), g(x, p)]_P$ between any pair of quantitates $f(x, p)$ and $g(x, p)$ in the following,

$$[f(x, p), g(x, p)]_D \equiv \[f(x, p), g(x, p)]_P - [f(x, p), \chi_\alpha(x, p)]_P C^{-1}_{\alpha\beta}[\chi_\beta(x, p), g(x, p)]_P,$$$$

where repeated indices are summed over in whole of this Letter, and $C_{\alpha\beta} \equiv [\chi_\alpha(x, p), \chi_\beta(x, p)]_P$ are the matrix elements in the constraint matrix $(C_{\alpha\beta})$ and the functions $\chi_\alpha(q, p)$ $(\alpha, \beta = 1, 2)$ are two constraints [38],

$$\chi_1(x, p) \equiv f(x) (= 0), \text{ and } \chi_2(x, p) \equiv n \cdot p (= 0).$$

II. DIRAC’S THEORY OF THE CONSTRAINED SYSTEMS: CLASSICAL AND QUANTUM MECHANICS

Let us consider a non-relativistically free particle that is constrained to remain on a surface described by a constraint in configurational space $f(x) = 0$, where $f(x)$ is some smooth function of position $x$, whose normal vector is $n \equiv \nabla f(x)$/$|\nabla f(x)|$. We can always choose the equation of the surface such that $|\nabla f(x)| = 1$, so that $n \equiv \nabla f(x)$. In classical mechanics, the Hamiltonian is simply $H = p^2/2\mu$ where $p$ denotes the momentum, and $\mu$ denotes the mass. However, in quantum mechanics, we cannot impose the usual canonical commutation relations $[x_i, p_j] = \pmih\delta_{ij}$, $(i, j = 1, 2, 3)$. Dirac was aware of the fact the presence of this constraint which needed to be eliminated before quantization could very well cause the remaining classical phase to not admit Cartesian coordinates.
A important property of vector $\mathbf{T}=d\mathbf{G}/dt$ is that it lies on the tangential surface, for we have $\mathbf{n} \cdot \mathbf{T}=0$. Relations (7)–(10) are revealing but somewhat trivial. In contrast, the consequence of these relations is significant in quantum mechanics, as we see shortly.

**B. Quantum conditions of the constrained system**

The scheme of the canonical quantization hypothesizes that in general the definition of a quantum commutator for any variables $f$ and $g$ is given by 

$$[f, g] = i\hbar O \{ [f, g] \}$$  \hfill (10)  

in which $O \{ f \}$ stands for the quantum operator corresponding to the classical quantity $f$. The *fundamental quantum conditions* are $[x_i, x_j]$, $[x_i, p_j]$ and $[p_i, p_j]$. For a particle moves in the free space, we have two fundamental operators in quantum mechanics, which in the configuration representation are position $\mathbf{x}$ and momentum $\mathbf{p} = -i\hbar \mathbf{\nabla}$. For a particle moves on a surface, there is in general a great difficulty in getting the momentum operator, because we run into the notorious operator-ordering difficulty of momentum and position operators in $O \{ (n_jn_i,k - n_in_j,k)p_k \} (= [p_i, p_j]/(i\hbar))$ from (7). Even worse is not the ambiguities in defining the Hamiltonian operator, but the Schrödinger-Podolsky-DeWitt approach is not able to give the correct form of the Hamiltonian operator no matter what form of the momentum operator is obtained. Thus, the commutators $[p_i, p_j]$ must be excluded from the so-called fundamental quantum conditions for they contain severe vagueness. Thus, we should search for *quantum conditions* beyond the usual fundamental ones. A straightforward enlargement of the quantum conditions is to simply follow the hypothesis given by (10) to include all $[f, H]$ as $f = \mathbf{x}$, $\mathbf{p}$ and $\mathbf{G}$ to simultaneously determine the operators $\mathbf{p}$ and $H$. It is fruitless at all, because there are much depressing operator-ordering difficulties in $O \{ \mathbf{n}(\mathbf{p} \cdot \mathbf{\nabla} \mathbf{n} \cdot \mathbf{p}) \} /\mu = (\mathbf{p} \cdot H)/(i\hbar)$ from (9) and $O \{ (\mathbf{x} \times \mathbf{n}) \mathbf{p} \cdot \mathbf{\nabla} \mathbf{n} \cdot \mathbf{p} \} /\mu = (\mathbf{G} \cdot H)/(i\hbar)$. To surmount these difficulties, we note following vanishing relations,

$$\mathbf{n} \cdot [\mathbf{x}, H] = \mathbf{n} \cdot \frac{\mathbf{p}}{\mu} = 0, \mathbf{n} \cdot [\mathbf{G}, H] = \mathbf{n} \cdot \mathbf{F} = 0 \text{ and } \mathbf{n} \times [\mathbf{p}, H] = 0.$$  \hfill (11)  

The resultant quantum conditions free from the operator-ordering difficulty are given by,

$$[x_i, x_j] = 0, \quad (12)$$

$$[x_i, p_j] = i\hbar (\delta_{ij} - n_jn_i), \quad (13)$$

$$[\mathbf{x}, H] = i\hbar \frac{\mathbf{p}}{\mu}, \quad (14)$$

$$\mathbf{n} \cdot [\mathbf{x}, H] + [\mathbf{x}, H] \cdot \mathbf{n} = i\hbar \frac{\mathbf{p}}{\mu} (\mathbf{n} \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{n}) = 0, \quad (15)$$

$$\mathbf{n} \times [\mathbf{p}, H] + [\mathbf{p}, H] \times \mathbf{n} = 0, \quad (16)$$

$$\mathbf{n} \cdot [\mathbf{G}, H] + [\mathbf{G}, H] \cdot \mathbf{n} = i\hbar (\mathbf{n} \cdot \mathbf{F} + \mathbf{F} \cdot \mathbf{n}) = 0. \quad (17)$$

The Hamiltonian operator must take the following form for it in classical limit reduces to the classical Hamiltonian $H = p^2/2\mu$,

$$H = -\frac{\hbar^2}{2\mu} \nabla_{LB}^2 + \alpha(x) \cdot \nabla_s + V_G,$$  \hfill (18)  

where $\alpha(x)$ and $V_G$ are functions that go over to zero not only in classical limit but also for free motion in flat space, which in general does not have an analog in classical mechanics, and $\nabla_{LB}^2 = \nabla_s \cdot \nabla_s$ is the Laplace-Beltrami operator which is the dot product of the gradient operator $\nabla_s$ on the surface.

The first condition (12) sets the configuration representation with Cartesian coordinates. The second condition (13) gives the essential part of the momentum $\mathbf{p}$ is the gradient $\nabla_s$ on the surface,

$$\mathbf{p} = -i\hbar (\nabla_s + \beta(x)), \quad (19)$$

where $\beta(x)$ is an undetermined vector function. Substituting (19) and (14) into the third condition (14), the momentum operator $\mathbf{p}$ and Hamiltonian operator $H$ becomes, respectively

$$\mathbf{p} = -i\hbar \left( \nabla_s + \frac{M}{2} \mathbf{n} \right). \quad (20)$$
where $M$ is a sum of two principal curvatures $R_{1}^{-1}$ and $R_{2}^{-1}$, $(R_{1}^{-1} + R_{2}^{-1})$ the mean curvature at point $x$ on the surface $S^2$

\[ H = \frac{\mu^2}{2\mu} + V_G - \hbar^2 M^2 \frac{2\mu}{8\mu}, \]  

(21)

where $\alpha(x) = 0$ in Eq. (13). It is easily to verify that the fourth and fifth conditions (14) and (15) are automatically satisfied whatever form of potential $V_G$ is. Lastly, let us calculate the $n \cdot [G, H] + [G, H] \cdot n$, and after a lengthy but straightforward manipulation, we arrive at,

\[ V_G = \frac{\hbar^2 M^2}{8\mu} - \frac{\hbar^2}{4\mu} (M^2 - 2K) + \varphi = -\frac{\hbar^2}{2\mu} \left\{ \left( \frac{M}{2} \right)^2 - K \right\} + \varphi, \]  

(22)

where $K$ is the gaussian curvature which is the product of the two principal curvatures as $(R_1 R_2)^{-1}$, and function $\varphi$ satisfies following differential equation,

\[ n \times \nabla \varphi = 0. \]  

(23)

It means that $\nabla \varphi$ is parallel to the normal direction $n = \nabla f(x)$, and we have $\nabla \varphi = \Phi(x)\nabla f(x)$ with $\Phi(x)$ being the magnitude of gradient of function $\varphi$. Since $|\nabla f(x)| = 1$, we have thus $\Phi(x) = \pm |\nabla \varphi|$. So, the function $\varphi$ defines a surface whose normal vectors is identical to the surface $f(x) = 0$. So, the new surface is identical to $f(x) = 0$, but takes another form $\varphi[f(x)] = 0$, i.e., we have $\varphi = 0$. The quantum Hamiltonian operator turns out to be,

\[ H = \frac{\mu^2}{2\mu} - \frac{\hbar^2}{2\mu} (M^2 - 2K) = -\frac{\hbar^2}{2\mu} \left( \nabla_{LB}^2 + \left( \frac{M}{2} \right)^2 - K \right). \]  

(24)

In the first expression, the curvature-induced potential is negative definite for we have $-\hbar^2/(2\mu) (R_1^{-2} + R_2^{-2})$, whereas in the second expression, the curvature-induced potential is semi-negative definite for we have $-\hbar^2/(8\mu) (R_1^{-1} - R_2^{-1})^2$, which is the so-called geometric potential,

\[ V_G = -\frac{\hbar^2}{2\mu} \left\{ \left( \frac{M}{2} \right)^2 - K \right\}. \]  

(25)

C. Further comments on the commutators $[p_i, p_j]$

The naive utilization of the relation (14), i.e., $O\{n_j n_{i, k} - n_i n_{j, k}\} = [p_i, p_j]/(i\hbar)$, is highly controversial topic to construct momentum. For instance, once can assume $O\{(n_j n_{i, k} - n_i n_{j, k})p_k\} \equiv c_1 n_j n_{i, k}p_k + c_2 p_k n_j n_{i, k} + c_3 n_j p_k n_{i, k} + c_4 n_{i, k} p_k n_j - (i \leftrightarrow j)$ where $c_1 + c_2 + c_3 + c_4 = 0$. But, because $n_j$ and $n_{i, k}$ contain various functions of coordinates of $x, y$ and $z$, e.g., we can have $n_j = x_j (x^2 + y^2 + z^2)^{-1/2}$, then operators $p_k n_j$ in the 4th term $n_{i, k} p_k n_j$ in above decomposition of $O\{(n_j n_{i, k} - n_i n_{j, k})p_k\}$ can at least be further decomposed as $p_k n_j = d_1 (x^2 + y^2 + z^2)^{-1/2} p_k x_j + d_2 x_j p_k (x^2 + y^2 + z^2)^{-1/2}$ where $d_1 + d_2 = 1$. No principle from either physics or mathematics can be used to terminate this procedure. So, the commutators $[p_i, p_j]$ can hardly be members of the fundamental quantum conditions. However, our geometric momentum turns out to satisfy the following relation,

\[ O\{(n_j n_{i, k} - n_i n_{j, k})p_k\} = \frac{1}{2} ((n_j n_{i, k} - n_i n_{j, k})p_k + p_k (n_j n_{i, k} - n_i n_{j, k})). \]  

(26)

Instead, our proposal is to reverse the quantization conditions $[p_i, p_j]/(i\hbar) = O\{(n_j n_{i, k} - n_i n_{j, k})p_k\}$ and to construct a function containing momentum operators such that we have,

\[ n \cdot P + P \cdot n = 0, \]  

(27)

where $P_j \equiv n \cdot [p, p_j] + [p, p_j] \cdot n$. Since this relation (27) alone is not yet able to give the momentum operators, we see that the commutators $[p_i, p_j]$ are not fundamental quantum conditions either.
III. CONCLUSIONS AND DISCUSSIONS

The quantum conditions given by the straightforward applications of the equation (10) are not always fruitful, even misleading. For the particle on the curved surface, in order to obtain the geometric potential predicted by the so-called thin-lay quantization, a proper enlargement of the quantum conditions turns out to be compulsory to contain positions, momenta, orbital angular momentum and Hamiltonian. What is more, a construction of unambiguous quantum conditions out of the equation (10) proves inevitable. Combining the enlargement and the construction, we obtain the geometric potential. Since momentum in the orbital angular momentum is the geometric one, which only in some special cases reduces to the usual one, we can call the orbital angular momentum the geometric angular momentum. Even the present paper deals with only the two-dimensional curved surface, we conjecture that our method can be used for particle on an arbitrarily dimensional curved surface, which is still under investigation.

Finally, we would like to point out that there are other forms of the enlargement and the construction in literature, for instance Refs. [42, 43], but they were devised to serve entirely different purposes.

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[1] B. S. DeWitt, Rev. Mod. Phys. 29, 377(1957).
[2] E. Schrödinger, Ann. Phys. (Leipzig), 79, 734(1926).
[3] B. Podolsky, Phys. Rev. 32, 812(1928).
[4] H. Jensen and H. Koppe, Ann. Phys. 63, 586(1971).
[5] R. C. T. da Costa, Phys. Rev. A 23, 1982(1981).
[6] A. V. Chaplik and R. H. Blick, New J. Phys. 6, 33(2004).
[7] M. V. Entin, and L. I. Magarill, Phys. Rev. B 64, 085330(2001)
[8] V. Atanasov, R. Dandoloff, and A. Saxena, Phys. Rev. B 79, 033404(2009).
[9] Y. N. Joglekar and A. Saxena, Phys. Rev. B 80, 153405(2009).
[10] S. Ono and H. Shima, Phys. Rev. B 79, 235407(2009).
[11] H. Shima, H. Yoshioka, and J. Onoe, Phys. Rev. B 79, 201401(2009).
[12] V. Atanasov and A. Saxena, Phys. Rev. B 81, 205409(2010).
[13] S. Ono, H. Shima, Physica E: Low Dimens. Syst. Nanostruct. 42, 1224–1227(2010)
[14] Y. Gaididei, V. P. Kravchuk, and D. D. Sheka, Phys. Rev. Lett. 112, 257203(2014).
[15] F. T. Brandt, J. A. Sánchez-Monroy, Europhys. Lett. 111, 67004(2015).
[16] C. Ortix and J. van den Brink, Phys. Rev. B 83, 113406(2011).
[17] D. Schmeltzer, J. Phys. Condens. Matter 23, 155601(2011).
[18] C. Filgueiras, E. O. Silva, Phys. Lett. A 379, 2110–2115(2015).
[19] N. Ogawa, Mod. Phys. Lett. A 12, 1583(1997).
[20] P. C. Schuster, and R. L. Jaffe, Ann. Phys. 307, 132-143(2003).
[21] A. Szameit, et. al, Phys. Rev. Lett. 104, 150403(2010).
[22] J. Onoe, T. Ito, H. Shima, H. Yoshioka, and S. Kimura, Europhys. Lett. 98, 27001(2012).
[23] Q. H. Liu, J. Phys. Soc. Jpn. 82, 104002(2013).
[24] P. A. M. Dirac, The Principles of Quantum Mechanics, 4th ed. (Oxford University Press, Oxford, 1967)P.114.
[25] P. A. M. Dirac, Lectures on quantum mechanics (Yeshiva University, New York, 1964); Can. J. Math. 2, 129(1950).
[26] J. Śniatycki, Geometric Quantumization and Quantum Mechanics (Springer–Verlag, New York, Heidelberg, Berlin, 1980)
[27] T. Homma, T. Inamoto, T. Miyazaki, Phys. Rev. D 42, 2049(1990).
[28] N. Ogawa, K Fujii and A. Kobushkin: Progress Theor. Phys. 83, 894(1990).
[29] N. Ogawa, K. Fujii, N. Chepilko and A. Kobushkin: Progress Theor. Phys. 85, 1189(1991).
[30] M. Isegami, Y. Nagaoka, S. Takagi, and T. Tanzawa, 88, 229(1992).
[31] M. Burgess and B. Jensen, Phys. Rev. A, 48, 1861(1993).
[32] C. Destri, P. Maraner, E. Onofri, Nuov. Cim. A, 107, 237(1994).
[33] H. Kleinert and S. V. Shabanov, Phys. Lett. A 232, 327(1997).
[34] E. A. Tagirov, arXiv:quant-ph/0101016-1 (2001).
[35] S. T. Hong, and K. D. Rothe, Ann. Phys. 311, 417–430(2004).
[36] A. V. Golovnev, Rep. Math. Phys. 64, 59(2009).
[37] B. Jensena, R. Dandoloff, Phys. Lett. A 375, 448-451(2011).
[38] S. Weinberg, Lectures on Quantum Mechanics, 2nd ed., (Cambridge University Press, Cambridge, 2015).
[39] Q.H. Liu, J. Math. Phys. 54, 122113(2013).
[40] Q.H. Liu, L.H. Tang, D.M. Xun, Phys. Rev. A 84, 042101(2011).
[41] Q. H. Liu, J. Zhang, D.K. Lian, L. D. Hu and Z. Li, Physica E: Low Dimens. Syst. Nanostruct. 87, 123(2017).
[42] C. M. Bender, and G. V. Dunne, Phys. Rev. D 40, 2739-2742(1989).
[43] A. Deriglazov, A. Nersessian, Phys. Lett A 378, 1224-1227(2014).