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Quantum Motion on 2D Surface of Nonspherical Topology

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An excess term exists when using hermitian form of Cartesian momentum $p_i (i = 1, 2, 3)$ in usual kinetic energy $1/(2\mu)\sum p_i^2$ for a particle moving on the 2D surface, and the correct kinetic energy turns to be $1/(2\mu)\sum 1/f_i p_i f_i p_i$ where the f_i are dummy factors in classical mechanics and nontrivial in quantum mechanics. In this paper, the explicit form of the dummy functions f_i is given for some surfaces of nonspherical topology, such as toroidal surface, paraboloid of revolution, the hyperboloid of revolution of two sheets, and the hyperboloid of revolution of one sheets.

KEY WORDS: quantum motion; nonspherical topology.

1. INTRODUCTION

Recently, we have noted that for a free particle moving on the surface of a sphere, or a rigid rotator, there is a new type of ordering problem with correct use of Cartesian momentum (Lia, 2003). In this paper, we will demonstrate that this problem presents in all constrained nonrelativistic quantum systems.

First, let us give a brief review of the ordering problem newly found in the rigid rotator. The quantum Hamiltonian for the rigid rotator is, (Cohen-Tannoudji, Diu, and Laloë, 1977),

$$T \equiv -\frac{\hbar^2}{2\mu}\nabla^2 = -\frac{\hbar^2}{2\mu r^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right) \tag{1}$$

This Hamiltonian can be obtained by canonical quantizations of classical Hamiltonian in either Cartesian-coordinate-dependent form T_{cc}

$$T_{cc} = \frac{1}{2\mu}\left(p_x^2 + p_y^2 + p_z^2\right) \tag{2}$$

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where μ is the reduced mass of the molecular system, or the generalized-coordinate-dependent form $T_{\rm gc}$ (Podolsky, 1928; Kleinert, 1990)

$$T_{\rm gc} = \frac{1}{2\mu}\sum_{ij}\frac{1}{g^{1/4}}p_i g^{1/4} g^{ij} g^{1/4} p_j \frac{1}{g^{1/4}} \tag{3}$$

where g_{ij} are the metric coefficients, g is the determinant of the g_{ij} matrix, and g^{ij} are the elements of inverse matrix of g_{ij}. To note that there is a dummy factor involving g in $T_{\rm gc}$, and these factors do not make sense unless in quantum mechanics (Podolsky, 1928; Kleinert, 1990) . However, different from the generalized momenta p_i used in $T_{\rm gc}$ (3) which are hermitian, the Cartesian momentum $p_i (i = 1, 2, 3)$ in $T_{\rm cc}$ (2) take the following *non-Hermitian* form

$$p_x = -i\hbar\frac{\partial}{\partial x} = -\frac{i\hbar}{r}\left(\cos\theta\cos\varphi\frac{\partial}{\partial\theta} - \frac{\sin\varphi}{\sin\theta}\frac{\partial}{\partial\varphi}\right) \tag{4}$$

$$p_y = -i\hbar\frac{\partial}{\partial y} = -\frac{i\hbar}{r}\left(\cos\theta\sin\varphi\frac{\partial}{\partial\theta} + \frac{\cos\varphi}{\sin\theta}\frac{\partial}{\partial\varphi}\right) \tag{5}$$

$$p_z = -i\hbar\frac{\partial}{\partial z} = -\frac{i\hbar}{r}\sin\theta\frac{\partial}{\partial\theta} \tag{6}$$

where the relations between Cartesian and spherical surface coordinates (x, y, z) and (θ, φ) are

$$x = r\sin\theta\cos\varphi, \quad y = r\sin\theta\sin\varphi, \quad z = r\cos\theta. \tag{7}$$

should take the following form

$$T = \sum_i \frac{1}{f_i(x, y, z)} p_{ih} f_i(x, y, z) p_{ih} \tag{15}$$

where $f_i(x, y, z)$ are dummy factors in classical mechanics, and whose existence can be easily demonstrated. The calculation of yielding an explicit form of function $f_i(x, y, z)$ in quantum mechanics is straightforward. In rest of this paper, we will list the results for some surfaces of nonspherical topology.

2. THE CORRECT USE OF HERMITIAN FORM OF CARTESIAN MOMENTUM IN QUANTUM MOTION CONSTRAINED ON 2D SURFACE OF NONSPHERICAL TOPOLOGY

2.1. The Quantum Motion on the Toroidal Surface

The toroidal surface is with two positive parameters (a, b) $(a \succ b)$,

$$\mathbf{Y} = ((a + b\sin\theta)\cos\varphi, (a + b\sin\theta)\sin\varphi, b\cos\theta)$$

where $\theta \in [0, 2\pi)$, $\varphi \in [0, 2\pi)$.

The kinetic energy operator reads [4],

$$T = -\frac{\hbar^2}{2m}\Delta = -\frac{\hbar^2}{2m}\left(\frac{1}{b^2}\frac{\partial^2}{\partial\theta^2} + \frac{1}{b^2}\frac{\partial \ln g}{\partial\theta}\frac{\partial}{\partial\theta} + \frac{1}{(a+b\sin\theta)^2}\frac{\partial^2}{\partial\varphi^2}\right) \quad (16)$$

where $g = b(a + b\sin\theta)$.

The Hermitian operators $p_i (i = 1, 2, 3)$ are,

$$p_x = -i\hbar\frac{1}{\sqrt{g}}\left(\frac{\partial}{\partial\theta}\sqrt{g}\frac{\cos\theta\cos\varphi}{b} + \frac{\partial}{\partial\varphi}\sqrt{g}\frac{\sin\varphi}{a+b\sin\theta}\right) \quad (17)$$

$$p_x = -i\hbar\frac{1}{\sqrt{g}}\left(\frac{\partial}{\partial\theta}\sqrt{g}\frac{\cos\theta\sin\varphi}{b} + \frac{\partial}{\partial\varphi}\sqrt{g}\frac{\cos\varphi}{a+b\sin\theta}\right) \quad (18)$$

$$p_x = -i\hbar\frac{1}{\sqrt{g}}\frac{\partial}{\partial\theta}\sqrt{g}\frac{\sin\theta}{b} \quad (19)$$

Then Eq. (15) holds true with $f_i(x, y, z)$ $(i = 1, 2, 3)$ being, respectively,

$$f_1(x, y, z) = \sqrt{yz}, \quad f_2(x, y, z) = \sqrt{xz},$$
$$f_3(x, y, z) = \sqrt[4]{(x^2 + y^2)(b^2 - z^2)} \quad (20)$$

This result reduces to that for the rigid rotator with $a = 0$, $b = r$.

2.2. The Quantum Motion on the Paraboloid of Revolution

The equation for the paraboloid of revolution is with a parameter η that can be conveniently chosen to be positive,

$$z = \frac{x^2 + y^2}{2\eta} - \frac{\eta}{2} \quad (21)$$

which can be rewritten in terms of parametric form,

$$x = \sqrt{\zeta\eta}\cos\varphi, \quad y = \sqrt{\zeta\eta}\sin\varphi, \quad z = \frac{1}{2}(\zeta - \eta) \quad (22)$$

where $\zeta \in (0, \infty)$ and $\varphi \in [0, 2\pi)$. The figure is shown in Fig. 1. The kinetic energy operator reads,

$$T = -\frac{\hbar^2}{2m}\Delta = -\frac{\hbar^2}{2m}\left(\frac{4}{g}\frac{\partial}{\partial\zeta}\frac{g\zeta}{(\zeta+\eta)}\frac{\partial}{\partial\zeta} + \frac{1}{\zeta\eta}\frac{\partial^2}{\partial\varphi^2}\right) \quad (23)$$

where $g = \sqrt{\eta(\zeta + \eta)}/2$. The hermitian operators $p_i (i = 1, 2, 3)$ are,

$$p_x = -i\hbar\frac{1}{\sqrt{g}}\left(\frac{\partial}{\partial\zeta}\sqrt{g}\frac{2\sin\varphi\sqrt{\zeta\eta}}{\zeta+\eta} - \frac{\partial}{\partial\varphi}\sqrt{g}\frac{\cos\varphi}{\sqrt{\zeta\eta}}\right) \quad (24)$$

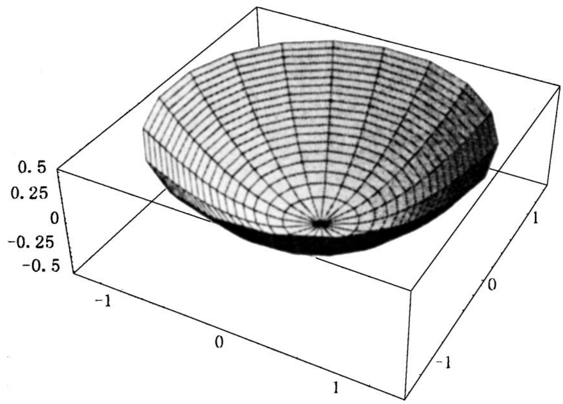

Fig. 1. The surface of paraboloid of revolution with parameter $\eta = 1$.

$$p_x = -i\hbar \frac{1}{\sqrt{g}} \left(\frac{\partial}{\partial \zeta} \sqrt{g} \frac{2 \sin \varphi \sqrt{\zeta \eta}}{\zeta + \eta} + \frac{\partial}{\partial \varphi} \sqrt{g} \frac{\cos \varphi}{\sqrt{\zeta \eta}} \right) \tag{25}$$

$$p_x = -i\hbar \frac{2}{\sqrt{g}} \frac{\partial}{\partial \zeta} \sqrt{g} \frac{\zeta}{\zeta + \eta} \tag{26}$$

Then Eq. (15) holds true with $f_i(x, y, z)$ $(i = 1, 2, 3)$ being, respectively,

$$f_1(x, y, z) = \left(\frac{\zeta \sin^2 \varphi}{\zeta + \eta} \right)^{1/4}, \quad f_2(x, y, z) = \left(\frac{\zeta \cos^2 \varphi}{\zeta + \eta} \right)^{1/4},$$
$$f_3(x, y, z) = \left(\frac{\zeta^2}{\zeta + \eta} \right)^{1/4} \tag{27}$$

2.3. The Quantum Motion on the Hyperboloid of Revolution of Two Sheets

The equation for the hyperboloid of revolution of two sheets is with parameter $\eta \in (-1, 1)$,

$$\frac{x^2 + y^2}{\eta^2} - \frac{z^2}{1 - \eta^2} = a^2 \tag{28}$$

which can also be rewritten in terms of parametric form,

$$x = a\zeta\eta \cos \varphi, \quad y = a\zeta\eta \sin \varphi, \quad z = a\sqrt{(\zeta^2 - 1)(1 - \eta^2)} \tag{29}$$

where $\zeta \in (1, \infty)$ and $\varphi \in [0, 2\pi)$ (see Fig. 2).

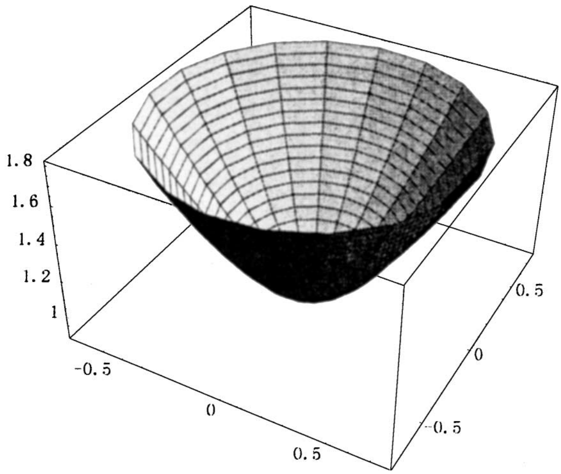

Fig. 2. The surface of hyperboloid of two sheets of revolution with parameters $a = 1$, $\eta = 0.7$.

The kinetic energy operator reads

$$T = -\frac{\hbar^2}{2m}\Delta = -\frac{\hbar^2}{2m}\left(\frac{1}{g}\frac{\partial}{\partial\zeta a^2}\frac{g(\zeta^2-1)}{(\zeta^2-\eta^2)}\frac{\partial}{\partial\zeta} + \frac{1}{a^2\zeta^2\eta^2}\frac{\partial^2}{\partial\varphi^2}\right) \tag{30}$$

where $g = a^2\zeta\eta\sqrt{(\zeta^2-\eta^2)/(\zeta^2-1)}$. The Hermitian operators $p_i (i = 1, 2, 3)$ are

$$p_x = -i\hbar\frac{1}{\sqrt{g}}\left(\frac{\partial}{\partial\zeta}\sqrt{g}\frac{\cos\varphi(\zeta^2-1)\eta}{a(\zeta^2-\eta^2)} + \frac{\partial}{\partial\varphi}\sqrt{g}\frac{\sin\varphi}{a\zeta\eta}\right) \tag{31}$$

$$p_x = -i\hbar\frac{1}{\sqrt{g}}\left(\frac{\partial}{\partial\zeta}\sqrt{g}\frac{\sin\varphi(\zeta^2-1)\eta}{a(\zeta^2-\eta^2)} + \frac{\partial}{\partial\varphi}\sqrt{g}\frac{\cos\varphi}{a\zeta\eta}\right) \tag{32}$$

$$p_x = -i\hbar\frac{1}{\sqrt{g}}\frac{\partial}{\partial\zeta}\sqrt{g}\frac{\zeta\sqrt{(\zeta^2-1)(1-\eta^2)}}{\zeta^2-\eta^2} \tag{33}$$

Then Eq. (15) holds true with $f_i(x, y, z)$ $(i = 1, 2, 3)$ being, respectively

$$f_1(x, y, z) = \left(\frac{\zeta^2\sin^2\varphi}{\zeta^2-\eta^2}\right)^{1/4}, \quad f_2(x, y, z) = \left(\frac{\zeta^2\cos^2\varphi}{\zeta^2-\eta^2}\right)^{1/4},$$

$$f_3(x, y, z) = \left(\frac{\zeta^4}{\zeta+\eta}\right)^{1/4} \tag{34}$$

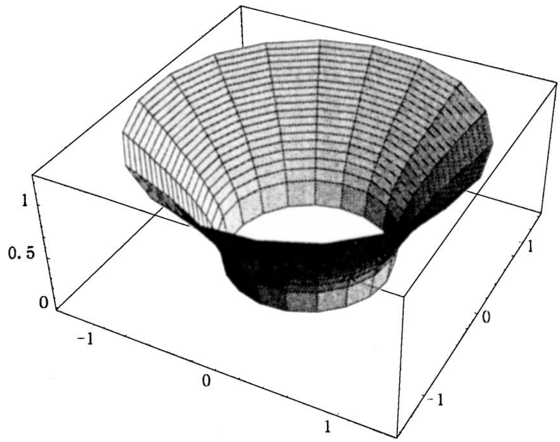

Fig. 3. The surface of hyperboloid of two sheets of revolution with parameters $a = 1$, $\eta = 0.7$.

2.4. The Quantum Motion on the Hyperboloid of Revolution of One Sheet

The equation for the hyperboloid of revolution of two sheets is with parameter $\eta \epsilon (-1, 1)$

$$-\frac{x^2 + y^2}{1 - \eta^2} + \frac{z^2}{\eta^2} = a^2 \tag{35}$$

which can also be rewritten in term of parametric form

$$x = a\sqrt{(\zeta^2 - 1)(1 - \eta^2)}\cos\varphi, \quad y = a\sqrt{(\zeta^2 - 1)(1 - \eta^2)}\sin\varphi, \quad z = a\zeta\eta \tag{36}$$

where parameter $\zeta \in (1, \infty)$, $\varphi \in [0, 2\pi)$ (see Fig. 3).

The kinetic energy operator reads

$$T = -\frac{\hbar^2}{2m}\Delta = -\frac{\hbar^2}{2m}\left(\frac{1}{g}\frac{\partial}{\partial\zeta}\frac{g(\zeta^2 - 1)}{a^2(\zeta^2 - \eta^2)}\frac{\partial}{\partial\zeta} + \frac{1}{a^2(\zeta^2 - 1)(1 - \eta^2)}\frac{\partial^2}{\partial\varphi^2}\right) \tag{37}$$

where $g = a^2\sqrt{(\zeta^2 - \eta^2)(\zeta^2 - 1)}$. The Hermitian operators $p_i (i = 1, 2, 3)$ are, respectively

$$p_x = -i\hbar\frac{1}{\sqrt{g}}\left(\frac{\partial}{\partial\zeta}\sqrt{g}\frac{\sin\varphi\zeta\sqrt{(\zeta^2 - \eta^2)(\zeta^2 - 1)}}{a(\zeta^2 - \eta^2)} - \frac{\partial}{\partial\varphi}\sqrt{g}\frac{\sin\varphi}{a\sqrt{(\zeta^2 - \eta^2)(\zeta^2 - 1)}}\right) \tag{38}$$

$$p_y = -i\hbar \frac{1}{\sqrt{g}} \left(\frac{\partial}{\partial \zeta} \sqrt{g} \frac{\sin\varphi \zeta \sqrt{(\zeta^2 - \eta^2)(\zeta^2 - 1)}}{a(\zeta^2 - \eta^2)} + \frac{\partial}{\partial \varphi} \sqrt{g} \frac{\cos\varphi}{a\sqrt{(\zeta^2 - \eta^2)(\zeta^2 - 1)}} \right) \tag{39}$$

$$p_x = -i\hbar \frac{1}{\sqrt{g}} \frac{\partial}{\partial \zeta} \sqrt{g} \frac{\eta(\zeta^2 - 1)}{a(\zeta^2 - \eta^2)} \tag{40}$$

Then Eq. (15) holds true with $f_i(x, y, z)$ $(i = 1, 2, 3)$ being, respectively

$$f_1(x, y, z) = \sqrt{\frac{g}{yz}}, \quad f_2(x, y, z) = \sqrt{\frac{g}{zx}}, \quad f_3(x, y, z) = \sqrt{\frac{g}{xy}} \tag{41}$$

3. CONCLUSION AND DISCUSSION

In this paper, we study in the 3D Cartesian coordinates the 2D geometrically constrained quantum systems. Results show that the quantum kinetic energy operators can be rewritten in the form of Eq. (15). We demonstrate through explicit functions that there is an ordering problem in it, i.e., the functions f_i in Eq. (15) is dummy in classical mechanics. This kind of ordering problem is entirely different from that in the existing one, the so-called correct quantum Hamiltonian operator written in an arbitrary curvilinear coordinate system (3). Our approach gives a new supporting of the completeness of theoretical frame of quantum mechanics.

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