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Quantum Motion on 2D Surfaces of Spherical Topology

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When the motion of a particle is constrained on the two-dimensional surface, excess terms exist in usual kinetic energy $1/(2\mu)\sum p_i^2$ with hermitian form of Cartesian momentum p_i $(i = 1, 2, 3)$, and the operator ordering should be taken into account in the kinetic energy which turns out to be $1/(2\mu)\sum(1/f_i)p_i f_i p_i$ where the functions f_i are dummy factors in classical mechanics and nontrivial in quantum mechanics. In this article, the explicit forms of the dummy functions f_i for quantum motion on some 2D surfaces of revolution of spherical topology are given.

KEY WORDS: quantum mechanics; canonical quantization.

PACS numbers: 03.65.-w Quantum mechanics, 04.60.Ds Canonical quantization.

Recently, we have noted that there is a new kind of constraint induced operator ordering (Lai *et al.*, 2006; Liu, 2006; Liu *et al.*, 2004; Liu and Liu, 2003; Xiao *et al.*, 2005). Since in majority of the realistic constraint problems the motion is on the 2-dimensional curved surfaces, for instance the ellipsoidal quantum dots, (Cantele *et al.*, 2001) this paper is going to present the detailed discussion on the constraint induced operator ordering for some typical 2D surfaces of spherical topology such as *ellipsoid surfaces and Spindle surfaces*.

The so-called constraint induced operator ordering arises from the applicability of the usual form of the kinetic energy operator,

$$T \equiv \frac{1}{2m}\left(p_x^2 + p_y^2 + p_z^2\right), \tag{1}$$

for the quantum motion constrained on the surface. When examining a constraint system in Cartesian coordinates with use of the hermitian form of Cartesian

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momentum p_i, we point out that the quantum kinetic energy operator (1) should be slightly generalized and take the following form (Lai *et al.*, 2006; Liu, 2006; Liu *et al.*, 2004; Liu and Liu, 2003; Xiao *et al.*, 2005).

$$T = \frac{1}{2m}\sum_{i=1}^{3}\frac{1}{f_i(x,y,z)}p_i f_i(x,y,z)p_i, \tag{2}$$

which differs from the usual form (1) in operator ordering (Kleinert, 1990) where f_i $(i = x, y, z)$ are non-trivial functions of three mutually dependent Cartesian coordinates. When the system is constraint-free, $f_i(x, y, z)$ become purely dummy; and the kinetic energy operator is reduced to be the usual form. The universality of the existence of such non-trivial functions f_i $(i = x, y, z)$ is proved in paper (Liu, 2006). In this article, we give the explicit forms of the dummy functions f_i $(i = x, y, z)$ for oblate, prolate ellipsoid surfaces and the spindle surfaces.

1, *Oblate ellipsoid surface* with two positive parameters (a, τ) $(\tau \succ 1, a \succ 0)$,

$$\frac{x^2+y^2}{\tau^2} + \frac{z^2}{\tau^2-1} = a^2. \tag{3}$$

It can also be paramerized by $\eta \in [-1, 1]$ and $\varphi \in [0, 2\pi)$ as

$$\mathbf{Y} = (a\eta\tau\cos\varphi, a\eta\tau\sin\varphi, a\sqrt{(\tau^2-1)(1-\eta^2)}). \tag{4}$$

The kinetic energy operator reads,

$$\begin{aligned} T &= -\frac{\hbar^2}{2m}\Delta \\ &= -\frac{\hbar^2}{2m}\frac{1}{a^2(\tau^2-\eta^2)}\left(\frac{\sqrt{1-\eta^2}}{\eta}\frac{\partial}{\partial\eta}\eta\sqrt{1-\eta^2}\frac{\partial}{\partial\eta} + \left(\frac{1}{\eta^2}+\frac{1}{\tau^2}\right)\frac{\partial^2}{\partial\varphi^2}\right). \end{aligned} \tag{5}$$

The hermitian operators p_i $(i = 1, 2, 3)$ are formed by Bohm's rule (Bohm, 1951):

$$p_i = \frac{1}{2}((-i\hbar\partial_i) + (-i\hbar\partial_i)^\dagger), (i = x, y, z). \tag{6}$$

Explicitly we have:

$$\begin{aligned} p_x = -i\hbar\frac{1}{a}&\left(\frac{(1-\eta^2)\tau\cos\varphi}{\tau^2-\eta^2}\frac{\partial}{\partial\eta} - \frac{\sin\varphi}{\eta\tau}\frac{\partial}{\partial\varphi}\right. \\ &\left. + \frac{1}{2\sqrt{g}}\left(\frac{\partial}{\partial\eta}\left(\sqrt{g}\frac{(1-\eta^2)\tau\cos\varphi}{\tau^2-\eta^2}\right) - \frac{\partial}{\partial\varphi}\left(\sqrt{g}\frac{\sin\varphi}{\eta\tau}\right)\right)\right), \end{aligned} \tag{7a}$$

$$p_y = -i\hbar\frac{1}{a}\left(\frac{(1-\eta^2)\tau\sin\varphi}{\tau^2-\eta^2}\frac{\partial}{\partial\eta}+\frac{\cos\varphi}{\eta\tau}\frac{\partial}{\partial\varphi}\right.$$
$$\left.+\frac{1}{2\sqrt{g}}\left(\frac{\partial}{\partial\eta}\left(\sqrt{g}\frac{\left(1-\eta^2\right)\tau\sin\varphi}{\tau^2-\eta^2}\right)+\frac{\partial}{\partial\varphi}\left(\sqrt{g}\frac{\cos\varphi}{\eta\tau}\right)\right)\right), \tag{7b}$$

$$p_z = -i\hbar\frac{1}{a}\left(\frac{\eta\sqrt{(1-\eta^2)\left(\tau^2-1\right)}}{\eta^2-\tau^2}\frac{\partial}{\partial\eta}\right.$$
$$\left.+\frac{1}{2\sqrt{g}}\frac{\partial}{\partial\eta}\left(\sqrt{g}\frac{\eta\sqrt{(1-\eta^2)\left(\tau^2-1\right)}}{\eta^2-\tau^2}\right)\right), \tag{7c}$$

where $\sqrt{g}=a^2\eta\tau\sqrt{(\tau^2-\eta^2)/(1-\eta^2)}$ comes from the invariant area element $\sqrt{g}d\eta d\varphi$ on the surface (4) and where the C-number terms with factor $1/(2\sqrt{g})$ come from the hermiticity requirement. However, if substituting p_i (7a)–(7c) into Eq. (1), we have excess terms in comparison with the standard form (5),

$$T+\frac{\hbar^2}{2m}\frac{1}{a^2(\tau^2-\eta^2)}\frac{(2\tau^2-\eta^2)(\tau^2-1)^2}{4\tau^2}. \tag{8}$$

In order to eliminate the excess terms, we resort to the dummy functions f_i $(i=x,y,z)$ (2). Then the explicit forms for f_i $(i=1,2,3)$ are respectively,

$$f_x = \frac{\eta^{C_1}(1-\eta^2)^{\frac{-1+2\tau^2-2C_1(\tau^2-1)}{4\tau^2}}}{(\tau^2-\eta^2)^{1/4}}\sin^{C_1}\varphi, \tag{9a}$$

$$f_y = \frac{\eta^{C_2}\left(1-\eta^2\right)^{\frac{-1+2\tau^2-2C_1\left(\tau^2-1\right)}{4\tau^2}}}{(\tau^2-\eta^2)^{1/4}}\cos^{C_2}\varphi, \tag{9b}$$

$$f_z = \frac{\eta}{(\tau^2-\eta^2)^{1/4}}. \tag{9c}$$

where C_1 and C_2 are two real numbers, and when $C_1=C_2=1/2$, we have simply,

$$f_x=\left(\frac{1-\eta^2}{\tau^2-\eta^2}\right)^{1/4}\sqrt{\eta\sin\varphi},\ f_y=\left(\frac{1-\eta^2}{\tau^2-\eta^2}\right)^{1/4}\sqrt{\eta\cos\varphi},\ f_z=\frac{\eta}{\left(\tau^2-\eta^2\right)^{1/4}}. \tag{10}$$

2, *Prolate ellipsoid surface* with two positive parameters (a,τ) $(\tau\succ 1, a\succ 0)$,

$$\frac{x^2+y^2}{\tau^2-1}+\frac{z^2}{\tau^2}=a^2. \tag{11}$$

It can also be paramerized by $\eta \in [-1, 1]$ and $\varphi \in [0, 2\pi)$ as

$$\mathbf{Y} =(a\sqrt{(\tau^2-1)(1-\eta^2)}\cos\varphi, a\sqrt{(\tau^2-1)(1-\eta^2)}\sin\varphi, a\eta\tau). \tag{12}$$

The kinetic energy operator reads,

$$\begin{aligned} T &= -\frac{\hbar^2}{2m}\Delta \\ &= -\frac{\hbar^2}{2m}\frac{1}{a^2(\tau^2-\eta^2)}\left(\frac{\partial}{\partial\eta}(1-\eta^2)\frac{\partial}{\partial\eta} + \left(\frac{1}{1-\eta^2} - \frac{1}{\tau^2-1}\right)\frac{\partial^2}{\partial\varphi^2}\right). \end{aligned} \tag{13}$$

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

$$\begin{aligned} p_x = -i\hbar\frac{1}{a}\Bigg(&-\frac{\eta\sqrt{(\tau^2-1)(1-\eta^2)}\cos\varphi}{\tau^2-\eta^2}\frac{\partial}{\partial\eta} - \frac{\sin\varphi}{\sqrt{(\tau^2-1)(1-\eta^2)}}\frac{\partial}{\partial\varphi} \\ &- \frac{1}{2\sqrt{g}}\left(\frac{\partial}{\partial\eta}\left(\sqrt{g}\frac{\eta\sqrt{(\tau^2-1)(1-\eta^2)}\cos\varphi}{\tau^2-\eta^2}\right) + \frac{\partial}{\partial\varphi}\left(\sqrt{g}\frac{\sin\varphi}{\sqrt{(\tau^2-1)(1-\eta^2)}}\right)\right)\Bigg), \end{aligned} \tag{14a}$$

$$\begin{aligned} p_y = -i\hbar\frac{1}{a}\Bigg(&-\frac{\eta\sqrt{(\tau^2-1)(1-\eta^2)}\sin\varphi}{\tau^2-\eta^2}\frac{\partial}{\partial\eta} + \frac{\cos\varphi}{\sqrt{(\tau^2-1)(1-\eta^2)}}\frac{\partial}{\partial\varphi} \\ &- \frac{1}{2\sqrt{g}}\left(\frac{\partial}{\partial\eta}\left(\sqrt{g}\frac{\eta\sqrt{(\tau^2-1)(1-\eta^2)}\sin\varphi}{\tau^2-\eta^2}\right) - \frac{\partial}{\partial\varphi}\left(\sqrt{g}\frac{\cos\varphi}{\sqrt{(\tau^2-1)(1-\eta^2)}}\right)\right)\Bigg), \end{aligned} \tag{14b}$$

$$p_z = -i\hbar\frac{1}{a}\left(\frac{\tau(1-\eta^2)}{\tau^2-\eta^2}\frac{\partial}{\partial\eta} + \frac{1}{2\sqrt{g}}\frac{\partial}{\partial\eta}\left(\sqrt{g}\frac{\tau(1-\eta^2)}{\tau^2-\eta^2}\right)\right), \tag{14c}$$

where $\sqrt{g} = a^2\sqrt{(\tau^2-\eta^2)(\tau^2-1)}$ comes from the invariant area element $\sqrt{g}d\eta d\varphi$ on the surface (12) and where the C-number terms with factor $1/(2\sqrt{g})$ come from the hermiticity requirement. However, if substituting p_i (14a)–(14c) into Eq. (1), we have an excess term in comparison with the standard form (13),

$$T + \frac{\hbar^2}{2m}\frac{\tau^2(\eta^2-2\tau^2+1)^2}{4a^2(\tau^2-\eta^2)^3(\tau^2-1)}. \tag{15}$$

In order to eliminate the excess terms, we resort to the dummy functions f_i $(i = x, y, z)$ (2). Then the explicit forms for f_i $(i = 1, 2, 3)$ are respectively,

$$f_x = \frac{\eta^{-\frac{2(C_1-1)\tau^2+1}{2(\tau^2-1)}}(1-\eta^2)^{C_1/2}}{(\tau^2-\eta^2)^{1/4}}\sin^{C_1}\varphi, \tag{16a}$$

$$f_y = \frac{\eta^{-\frac{2(C_2-1)\tau^2+1}{2(\tau^2-1)}}(1-\eta^2)^{C_2/2}}{(\tau^2-\eta^2)^{1/4}}\cos^{C_2}\varphi, \tag{16b}$$

$$f_z = \frac{(1-\eta^2)^{1/2}}{(\tau^2-\eta^2)^{1/4}}. \tag{16c}$$

where C_1 and C_2 are two real numbers, and when $C_1 = C_2 = 1/2$, we have simply,

$$f_x = \left(\frac{1-\eta^2}{\tau^2-\eta^2}\right)^{1/4} \sqrt{\eta \sin\varphi},\ f_y = \left(\frac{1-\eta^2}{\tau^2-\eta^2}\right)^{1/4} \sqrt{\eta \cos\varphi},\ f_z = \frac{\left(1-\eta^2\right)^{1/2}}{\left(\tau^2-\eta^2\right)^{1/4}}. \tag{17}$$

3, *Spindle surface* can be parameterized by $\eta \in (-\infty, \infty)$ and $\varphi \in [0, 2\pi)$ as:

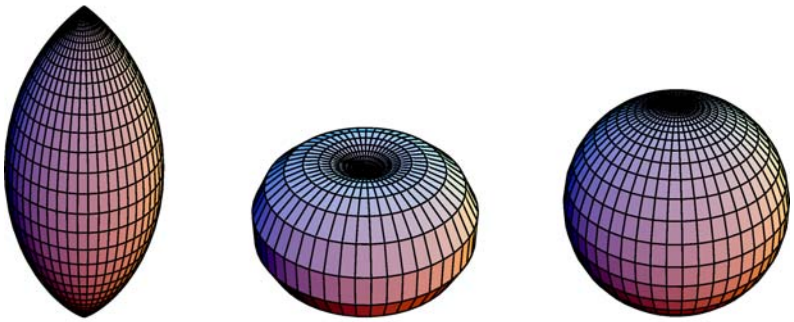
$$\mathbf{Y} = \left(\frac{a \sin\tau}{\cosh\eta - \cos\tau}\cos\varphi, \frac{a\sin\tau}{\cosh\eta - \cos\tau}\sin\varphi, \frac{a\sinh\eta}{\cosh\eta-\cos\tau}\right) \tag{18}$$

where a is a positive number and τ is a parameter and when $\tau \succ \pi/2$, $\tau \prec \pi/2$ and $\tau = \pi/2$, the spindles have outward corners and inward corners and takes the perfect sphere respectively, as shown in (a), (b) and (c) in Fig. 1. The kinetic energy operator reads,

$$\begin{aligned} T &= -\frac{\hbar^2}{2m}\Delta \\ &= -\frac{\hbar^2}{2m}\frac{(\cosh\eta-\cos\tau)^2}{a^2}\left((\cosh\eta-\cos\tau)\frac{\partial}{\partial\eta}\frac{1}{(\cosh\eta-\cos\tau)}\frac{\partial}{\partial\eta} + \frac{1}{\sin^2\tau}\frac{\partial^2}{\partial\varphi^2}\right). \end{aligned} \tag{19}$$

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

$$\begin{aligned} p_x = -i\hbar\frac{1}{a}\Bigg(&-\sin\tau\sinh\eta\cos\varphi\frac{\partial}{\partial\eta} + \frac{\cos\tau-\cosh\eta}{\sin\tau}\sin\varphi\frac{\partial}{\partial\varphi} \\ &- \frac{1}{2\sqrt{g}}\left(\frac{\partial}{\partial\eta}(\sqrt{g}\sin\tau\sinh\eta\cos\varphi) - \frac{\partial}{\partial\varphi}\left(\sqrt{g}\frac{\cos\tau-\cosh\eta}{\sin\tau}\sin\varphi\right)\right)\Bigg), \end{aligned} \tag{20a}$$



(a) (b) (c)

Fig. 1. Spindles with $\tau = 3\pi/4$ (a), $\pi/4$ (b) which have outward and inward corners at two poles respectively. When $\tau = \pi/2$ (c), the spindle gives a sphere.

$$p_y = -i\hbar\frac{1}{a}\left(-\sin\tau\sinh\eta\sin\varphi\frac{\partial}{\partial\eta} - \frac{\cos\tau - \cosh\eta}{\sin\tau}\cos\varphi\frac{\partial}{\partial\varphi}\right.$$
$$\left. - \frac{1}{2\sqrt{g}}\left(\frac{\partial}{\partial\eta}(\sqrt{g}\sin\tau\sinh\eta\sin\varphi) + \frac{\partial}{\partial\varphi}\left(\sqrt{g}\frac{\cos\tau - \cosh\eta}{\sin\tau}\cos\varphi\right)\right)\right), \quad (20b)$$

$$p_z = -i\hbar\frac{1}{a}\left((1 - \cos\tau\cosh\eta)\frac{\partial}{\partial\eta} + \frac{1}{2\sqrt{g}}\frac{\partial}{\partial\eta}(\sqrt{g}(1 - \cos\tau\cosh\eta))\right), \quad (20c)$$

where $\sqrt{g} = a^2\sin\tau/(\cos\tau - \cosh\eta)^2$ comes from the invariant area element $\sqrt{g}d\eta d\varphi$ on the surface (18) and where there C-number terms with factor $1/(2\sqrt{g})$ come from the hermiticity requirement. However, if substituting p_i (14a)–(14c) into Eq. (1), we have excess terms in comparison with the standard form (19),

$$T + \frac{\hbar^2}{2m}\frac{(3 - \cos 2\tau - 2\cos\tau\cosh\eta)^2}{16a^2\sin^2\tau}. \quad (21)$$

In order to eliminate the excess terms, we resort to the dummy functions f_i $(i = x, y, z)$ (2). Then the explicit forms for f_i $(i = 1, 2, 3)$ are respectively,

$$f_x = \frac{(\sinh\eta)^{\frac{1}{2}((1-2C_1)\csc^2\tau+1)}(\tanh\frac{\eta}{2})^{\frac{1}{2}(2C_1-1)\cot\tau\csc\tau}}{\cos\tau - \cosh\eta}\sin^{C_1}\varphi, \quad (22a)$$

$$f_y = \frac{(\sinh\eta)^{\frac{1}{2}((1-2C_2)\csc^2\tau+1)}(\tanh\frac{\eta}{2})^{\frac{1}{2}(2C_2-1)\cot\tau\csc\tau}}{\cos\tau - \cosh\eta}\cos^{C_2}\varphi, \quad (22b)$$

$$f_z = \frac{\sqrt{1 - \cos\tau\cosh\eta}}{\cos\tau - \cosh\eta}. \quad (22c)$$

where C_1 and C_2 are two real numbers, and when $C_1 = C_2 = 1/2$, we have simply,

$$f_x = \frac{\sqrt{\sinh\eta\sin\varphi}}{\cos\tau - \cosh\eta}, f_y = \frac{\sqrt{\sinh\eta\cos\varphi}}{\cos\tau - \cosh\eta}, f_z = \frac{\sqrt{1 - \cos\tau\cosh\eta}}{\cos\tau - \cosh\eta}. \quad (23)$$

It is also easy to prove that when $\tau = \pi/2$, f_i (22a)–(22c) reduce to those for sphere, (Liu, 2006; Liu and Liu, 2003) as they should be.

Before enclosing this article, we like to make following comments. This kind of ordering problem is entirely different from the well-known one, the so-called correct quantum Hamiltonian operator written in an arbitrary curvilinear coordinate system, (Kleinert, 1990) and our ordering problem completely arises from the constraint. This new ordering problem and its solution offer a new evidence showing the self-consistence of quantum mechanics using the naive definition for hermitian operator (Bohm, 1951).

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