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Universality of Operator Ordering in Kinetic Energy Operator for Particles Moving on two Dimensional Surfaces

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When the motion of a particle is constrained on the two-dimensional surface, excess terms exist in usual kinetic energy $1/(2m)\sum p_i^2$ 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 $1/(2m)\sum(1/f_i)p_i f_i p_i$ where the functions f_i are dummy factors in classical mechanics and nontrivial in quantum mechanics. The existence of non-trivial f_i shows the universality of this constraint induced operator ordering in quantum kinetic energy operator for the constraint systems.

KEY WORDS: quantum mechanics; canonical quantization.

Recently, the physics of nanostructures and quantum waveguides pose questions concerning curved surfaces in quantum theory (Encinosa and Mott, 2003). On the kinetic side, the common thread through much of the work is the existence of an attractive potential that appears in the Schrödinger equation as a consequence of constraining a particle from higher- to lower dimensional manifolds (Encinosa and Mott, 2003). On the kinematic side, a reasonable question raised is whether we can still use the usual form of the kinetic energy operator,

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

In fact, in majority of the realistic constraint problems, the motion is on the 2-dimensional curved surface. When examining a constraint system in Cartesian coordinates with use of the hermitian form of Cartesian momentum p_i, the quantum kinetic energy operator (1) should be slightly generalized and take the following form (Liu and Liu, 2003; Liu *et al.*, 2004; Xiao *et al.*, 2005)

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

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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 and the subscripts i, denoted by Latin letters, are always referred to x, y, z when $i = 1, 2, 3$ respectively. When the system is constraint-free, $f_i(x, y, z)$ become dummy; and the kinetic energy operator is reduced to be the usual form. The presence of the non-trivial functions f_i ($i = x, y, z$) is a new kind of operator ordering induced by the constraint.

For the particle moves on the curved surface which is parameterized by two independent local coordinates (u, v), the kinetic energy takes the following form

$$T \equiv -\frac{\hbar^2}{2m}\nabla^2 = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right). \tag{3}$$

The differential operators $\partial_i \equiv \partial/\partial x_i$ $(i = 1, 2, 3)$, which are not independent from each other, can be expressed in terms of the combination of $\partial/\partial u$ and $\partial/\partial v$ which are explicitly

$$\partial_i = X_{i\alpha}\partial_\alpha, \tag{4}$$

where $\partial_\alpha = \partial/\partial u$ and $\partial/\partial v$ respectively and Greek letters α and β are used to mean u, v on the surface, and $X_{i\alpha} \equiv X_{i\alpha}(u, v)$ are transformation coefficients. Hereafter, the convention is used that the repeated indices mean summation unless specified. For simplicity, we will use unit in which $\hbar^2/(2m) = 1$. So we have from Eq. (3),

$$T = -\partial_i^2 = -X_{i\alpha}\partial_\alpha X_{i\beta}\partial_\beta. \tag{5}$$

To note that the operators $-i\partial_i$ are no longer hermitian, but the hermitian operators can be easily formed by the Bohm's rule (Bohm, 1951) and they are

$$\begin{aligned} p_i &\equiv \frac{1}{2}\left\{(-i\hbar\partial_i + (-i\hbar\partial_i)^\dagger\right\} \\ &= -i\hbar\left\{X_{i\alpha}\partial_\alpha + \frac{1}{2\sqrt{g}}\partial_\alpha(\sqrt{g}X_{i\alpha})\right\} \\ &= -i\hbar\left\{X_{i\alpha}\partial_\alpha + \Pi_i\right\}, \qquad (i = 1, 2, 3). \end{aligned} \tag{6}$$

where $g = \det(g_{\alpha\beta})$ is the determinant of the metric coefficient matrix $g_{\alpha\beta}$ which is defined via the length element square $ds^2 = g_{\alpha\beta}du^\alpha du^\beta$ on the surface and$\sqrt{g}\,du\,dv$ is the area element, and $\Pi_i \equiv \frac{1}{2\sqrt{g}}\partial_\alpha(\sqrt{g}X_{i\alpha})$. Substituting p_i into Eq. (2), we have

$$\begin{aligned} T &= \frac{1}{2m}\frac{1}{f_i(x, y, z)}p_i f_i(x, y, z)p_i \\ &= -\left(\frac{1}{f_i}X_{i\alpha}\partial_\alpha f_i + \Pi_i\right)(X_{i\beta}\partial_\beta + \Pi_i) \end{aligned}$$

$$= -\left(X_{i\alpha}\partial_\alpha + \Pi_i + \frac{1}{f_i} X_{i\alpha}(\partial_\alpha f_i) \right) (X_{i\beta}\partial_\beta + \Pi_i)$$
$$= -(X_{i\alpha}\partial_\alpha + \Pi_i + \Xi_i)(X_{i\beta}\partial_\beta + \Pi_i), \tag{7}$$

where $f_i = f_i(u, v)$ are functions of two independent variables u and v, and

$$\Xi_i \equiv \frac{1}{f_i} X_{i\alpha}(\partial_\alpha f_i), \text{ (no summation over three repeated indices } i). \tag{8}$$

Then, to prove that the universality of the constraint induced operator ordering amounts to prove the following mathematical theorem:

Theorem 1. *The non-trivial functions f_i $(i = x, y, z)$ in Eq. (2) or in Eq. (7) exist in general.*

Proof: Expanding the right hand side of Eq. (7), we find

$$\begin{aligned} T &= -(X_{i\alpha}\partial_\alpha + \Pi_i + \Xi_i)\ (X_{i\beta}\partial_\beta + \Pi_i) \\ &= -(X_{i\alpha}\partial_\alpha X_{i\beta}\partial_\beta + (X_{i\alpha}\partial_\alpha \Pi_i + \Pi_i X_{i\beta}\partial_\beta) + \Pi_i^2 + \Xi_i(X_{i\beta}\partial_\beta + \Pi_i)) \\ &= -(X_{i\alpha}\partial_\alpha X_{i\beta}\partial_\beta + \left\{(2\Pi_i + \Xi_i)X_{i\beta}\right\}\partial_\beta + \{X_{i\alpha}(\partial_\alpha \Pi_i) + \Xi_i \Pi_i + \Pi_i \Pi_i\}). \end{aligned} \tag{9}$$

Evidently, if f_i-dependent term Ξ_i is absent from above Eq. (9), there are excess terms $2\Pi_i X_{i\beta}\partial_\beta + X_{i\alpha}(\partial_\alpha \Pi_i) + \Pi_i \Pi_i$ in (9) in comparison with the correct kinetic operator (5). On the other hand, the presence of f_i-dependent term Ξ_i may cancel out the excess terms, making the terms in two parenthesis {} in (9) vanish. This requirement leads to the following three equations,

$$(2\Pi_i + \Xi_i)X_{i\alpha} = 0, (\alpha = u, v), \tag{10}$$

$$X_{i\alpha}(\partial_\alpha \Pi_i) + \Xi_i \Pi_i + \Pi_i \Pi_i = 0. \tag{11}$$

Associating these three equations, we can obtain the solutions for Ξ_i,

$$\vec{\Xi} = \frac{-(\vec{X_\alpha} \cdot \partial_\alpha \vec{\Pi} + \vec{\Pi} \cdot \vec{\Pi})\vec{X_u} \times \vec{X_v} + 2(\vec{\Pi} \cdot \vec{X_u})(\vec{\Pi} \times \vec{X_v}) + 2(\vec{\Pi} \cdot \vec{X_v})(\vec{X_u} \times \vec{\Pi})}{(\vec{X_u} \times \vec{X_v}) \cdot \vec{\Pi}}, \tag{12}$$

where

$$\vec{X_\alpha} = (X_{x\alpha}, X_{y\alpha}, X_{z\alpha}), (\alpha = u, v). \tag{13}$$

Equations (12) are in fact three independent first-order partial differential equations determining f_i respectively which are involved in Ξ_i (8), and how to obtain their solutions is elementary (Kevorkian, 2000). From the existence theorem of the non-trivial solutions to the first-order partial differential equation (Kevorkian, 2000), the universality of the existence holds for the constraint induced operator ordering in Eq. (2) or in Eq. (7). □

In the following, the closed form for f_i for two constraint systems is explicitly given 1.

For a particle moves on the surface of a sphere of radius r, (Liu and Liu, 2003)

$$x = r\sin\theta\ \cos\varphi, \qquad y = r\sin\theta\ \sin\varphi, \qquad z = r\cos\theta, \tag{14}$$

the hermitian operators for Cartesian momenta p_i are respectively,

$$p_x = -\frac{i\hbar}{r}\left(\cos\theta\ \cos\varphi\frac{\partial}{\partial\theta} - \frac{\sin\varphi}{\sin\theta}\frac{\partial}{\partial\varphi} - \sin\theta\ \cos\varphi\right), \tag{15}$$

$$p_y = -\frac{i\hbar}{r}\left(\cos\theta\ \sin\varphi\frac{\partial}{\partial\theta} + \frac{\cos\varphi}{\sin\theta}\frac{\partial}{\partial\varphi} - \sin\theta\ \sin\varphi\right), \tag{16}$$

$$p_z = \frac{i\hbar}{r}\left(\sin\theta\frac{\partial}{\partial\theta} + \cos\theta\right). \tag{17}$$

The three first order linear partial differential Eq. (12) become,

$$\partial_\theta f_x(\theta,\varphi) - \csc\theta\ \sec\theta\ \tan\varphi\partial_\varphi f_x(\theta,\varphi) + \tan\theta\ f_x(\theta,\varphi) = 0, \tag{18}$$

$$\partial_\theta f_y(\theta,\varphi) + \cot\varphi\ \csc\theta\ \sec\theta\ \partial_\varphi f_y(\theta,\varphi) + \tan\theta\ f_z(\theta,\varphi) = 0, \tag{19}$$

$$\partial_\theta f_z(\theta,\varphi) - \cot\varphi f_z(\theta,\varphi) = 0. \tag{20}$$

whose general solutions are,

$$\begin{aligned} f_x(\theta,\varphi) &= \cos^{1-\alpha}\theta\sin^{\alpha}\theta\sin^{\alpha}\varphi, \\ f_y(\theta,\varphi) &= \cos^{1-\beta}\theta\sin^{\beta}\theta\cos^{\beta}\varphi, \\ f_z(\theta,\varphi) &= \sin\theta, \end{aligned} \tag{21}$$

where α and β are two real constants.

2, For a particle which moves on the surface of the torus (Encinosa and Mott 2003; Liu *et al.* 2004). The toroidal surface is with two positive parameters (a, b) $(a \succ b)$(Encinosa and Mott, 2003; Liu *et al.*, 2004),

$$x = (a + b\sin\theta)\cos\varphi, \qquad y = (a + b\sin\theta)\sin\varphi, \qquad z = b\cos\theta \tag{22}$$

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

The hermitian operators for Cartesian momenta p_i are respectively,

$$\begin{aligned} p_x = &-i\hbar\left(\frac{\cos\theta\ \cos\varphi}{b}\frac{\partial}{\partial\theta} - \frac{\sin\varphi}{a + b\ \sin\theta}\frac{\partial}{\partial\varphi}\right) \\ &-i\hbar\frac{1}{2\sqrt{g}}\left(-\frac{\partial}{\partial\theta}\left(\sqrt{g}\frac{\cos\theta\ \cos\varphi}{b}\right) - \frac{\partial}{\partial\varphi}\left(\sqrt{g}\frac{\sin\varphi}{a + b\ \sin\theta}\right)\right), \end{aligned} \tag{23}$$

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

$$p_x = i\hbar\frac{\sin\theta}{b}\frac{\partial}{\partial\theta} + i\hbar\frac{1}{2\sqrt{g}}\frac{\partial}{\partial\theta}\left(\sqrt{g}\frac{\sin\theta}{b}\right). \quad (25)$$

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

The three first order linear partial differential Eqs. (12) become,

$$(a + b\,\sin\theta)\partial_\theta f_x(\theta,\varphi) - b\,\sec\theta\,\tan\varphi\,\partial_\varphi f_x(\theta,\varphi) + \frac{1}{2}f_x(\theta,\varphi)(a + 2b\,\sin\theta)\tan\theta = 0, \quad (26)$$

$$(a + b\,\sin\theta)\partial_\theta f_y(\theta,\varphi) + b\,\sec\theta\,\cot\varphi\,\partial_\varphi f_x(\theta,\varphi) - \frac{1}{2}f_y(\theta,\varphi)(a + 2b\,\sin\theta)\tan\theta = 0, \quad (27)$$

$$(a + b\,\sin\theta)\partial_\theta f_z(\theta,\varphi) - \frac{1}{2}f_z(\theta,\varphi)(a + 2b\,\sin\theta)\cot\theta = 0. \quad (28)$$

whose general solutions are,

$$f_x(\theta,\varphi) = \sin^\beta\varphi\left(\cos\frac{\theta}{2} - \sin\frac{\theta}{2}\right)^{(a-2\,b\,(-1+\alpha))/2\,(a+b)} \times \left(\cos\frac{\theta}{2} + \sin\frac{\theta}{2}\right)^{(a-2\,b+2\,b\,\alpha)/2\,(a-b)} (a + b\,\sin\theta)^{(a^2-2\,b^2\,\alpha)/2(a^2-b^2)}, \quad (29)$$

$$f_y(\theta,\varphi) = \cos^\beta\varphi\left(\cos\frac{\theta}{2} - \sin\frac{\theta}{2}\right)^{(a-2\,b\,(-1+\alpha))/2\,(a+b)} \times \left(\cos\frac{\theta}{2} + \sin\frac{\theta}{2}\right)^{(a-2\,b+2\,b\,\alpha)/2(a-b)} (a + b\,\sin\theta)^{(a^2-2\,b^2\,\alpha)/2(a^2-b^2)}, \quad (30)$$

$$f_z(\theta,\varphi) = \sqrt{(a + b\sin\theta)\sin\theta}, \quad (31)$$

where α and β are two real constants. When $a = 0$, all results from (22) to (31) for toroidal surface reduce to be those for spherical surface, as they must be. When $\alpha = \beta = 1/2$, the functions $f_i(\theta,\varphi)$ take the following simple forms from (29)–(31),

$$f_x(\theta,\varphi) = \sqrt{(a + b\sin\theta)\cos\theta\,\sin\varphi} = \sqrt{yz/b}, \quad (32)$$

$$f_y(\theta,\varphi)=\sqrt{(a+b\sin\theta)\cos\theta\cos\varphi}=\sqrt{xz/b}, \tag{33}$$

$$\begin{aligned} f_z(\theta,\varphi)&=\sqrt{(a+b\sin\theta)(a+b\sin\theta-a)/b}\\ &=\sqrt{\sqrt{(x^2+y^2)}(\sqrt{(x^2+y^2)}-a)/b}, \end{aligned} \tag{34}$$

where mapping from (u, v) to (x, y, z) (22) is used. From Eqs. (32)–(34), we see clearly that once the constraint is absent, f_i and Cartesian momentum p_i are mutually commutable $[f_i, p_i]=0$. Thus the Eq. (2) reproduces Eq. (1).

Before enclosing this short paper, 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 (Podolsky, 1928; 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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