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Quantum Hamiltonian for the Rigid Rotator

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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 the rigid rotator, and the correct kinetic energy turns to be $1/(2\mu)\sum(1/f_i)p_i f_i p_i$ where f_i are dummy factors in classical mechanics and nontrivial in quantum mechanics.

KEY WORDS: quantum Hamiltonian; rigid rotator.

A free particle on the surface of a sphere, or a rigid rotator, is an ideal physical system modeling the rotation of two nuclei about their center of mass for a diatomic molecule. Every physics undergraduate should learn how to treat this system in his elementary quantum mechanics course, and he can then find the correct result for the heat capacity and other physics properties of the diatomic molecule gas. As well-known, the quantum Hamiltonian for the rigid rotator is (Cohen-Tannoudji *et al.*, 1977),

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

where μ is the reduced mass of the molecular system. The eigenfunctions are usual spherical harmonics $|l, m\rangle$ and eigenvalues are essentially those of the square of angular momentum $l(l+1)\hbar^2/(2\mu r^2)$ $(l = 0, 1, 2, \ldots)$ (Cohen-Tannoudji *et al.*, 1977). However, this is a constrained system. In this article, we are going to demonstrate that an operator ordering problem presents with the Cartesian coordinates, and how this problem is resolved by an appropriate ordering of the Cartesian coordinates and Cartesian momenta in the quantum Hamiltonian

The Hamiltonian (1) can be obtained by canonical quantization. However, the classical Hamiltonian has two equivalent forms:

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(1) The Cartesian-coordinate-dependent form,

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

(2) The generalized-coordinate-dependent form,

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

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}. Note that there are dummy factors involving g in T_{gc}, and these factors do not make sense except in quantum mechanics, as was first observed by Podolsky (1928). In quantum mechanics, these two forms (2) and (3) are identical provided that the system is unconstrained. However, for the motion of the particle moving on the surface of the sphere of fixed radius r which is constrained, Eqs. (2) and (3) in quantum mechanics are no longer equivalent to each other. On one hand, the Cartesian momentum p_i ($i = 1, 2, 3$) in T_{cc} 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 $(0, \varphi)$ are

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

However, the hermitian operators p_{ih} for $-i\hbar\partial_i$ (4)–(6) can be easily formed by use of the Bohm's rule $1/2(-i\hbar\partial_i + (-i\hbar\partial_i)^{\dagger})$, and results are

$$p_{xh} = -\frac{i\hbar}{r}\left(\cos\theta\ \cos\varphi\frac{\partial}{\partial\theta} - \frac{\sin\varphi}{\sin\theta}\frac{\partial}{\partial\varphi} - \sin\theta\ \cos\varphi\right), \tag{8}$$

$$p_{yh} = -\frac{i\hbar}{r}\left(\cos\theta\ \sin\varphi\frac{\partial}{\partial\theta} + \frac{\cos\varphi}{\sin\theta}\frac{\partial}{\partial\varphi} - \sin\theta\ \sin\varphi\right), \tag{9}$$

$$p_{zh} = -\frac{i\hbar}{r}\left(\sin\theta\frac{\partial}{\partial\theta} + \cos\theta\right). \tag{10}$$

On the other hand, the generalized momentum p_i in spherical polar coordinates (3) take the following *hermitian* form (Kleinert, 1990),

$$p_\theta = -i\hbar \frac{1}{\sqrt{\sin\theta}} \frac{\partial}{\partial\theta} \sqrt{\sin\theta}, \qquad p_\varphi = -i\hbar \frac{\partial}{\partial\varphi}. \tag{11}$$

An intriguing question is why we cannot use the hermitian form of the Cartesian momentum p_{ih} in $T_{\rm cc}$ and what will happen if one insists on using p_{ih} rather than $-i\hbar\partial_i$ in it. As far as we know, no literature discusses this question. In fact, there is also an ordering problem. If inserting p_{ih} instead of $-i\hbar\partial_i$ into Eq. (2), we find

$$T_{\rm new} = \frac{1}{2\mu}\left(p_{xh}^2 + p_{yh}^2 + p_{zh}^2\right) \tag{12}$$

$$= \frac{\hbar^2}{2\mu r^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right) + \frac{\hbar^2}{2\mu r^2} = T + \frac{\hbar^2}{2\mu r^2}, \tag{13}$$

which is wrong for there is an excess term $\hbar^2/(2\mu r^2)$. To obtain correct result, we should insert some dummy factors in Eq. (12). The possibly simplest choice of the dummy factors turns out to be

$$T = \frac{1}{2\mu}\left(\frac{1}{\sqrt{yz}} p_{xh}\sqrt{yz}\, p_{xh} + \frac{1}{\sqrt{zx}} p_{yh}\sqrt{zx}\, p_{yh} + \frac{1}{\sqrt{xy}} p_{zh}\sqrt{xy}\, p_{zh}\right) \tag{14}$$

$$= -\frac{\hbar^2}{2\mu}\nabla^2. \tag{15}$$

We can carry out the general dummy factors in Eqs. (12) and (14) as

$$\begin{aligned} T = \frac{1}{2\mu}\Bigg(& \frac{1}{\sin^\alpha\theta\,\cos^{1-\alpha}\theta\,\sin^\alpha\varphi} p_{xh}\,\sin^\alpha\theta\,\cos^{1-\alpha}\theta\,\sin^\alpha\varphi p_{xh} \\ & + \frac{1}{\sin^\beta\theta\,\cos^{1-\beta}\theta\,\sin^\beta\varphi} p_{yh}\,\sin^\beta\theta\,\cos^{1-\beta}\theta\,\sin^\beta\varphi p_{yh} \\ & + \frac{1}{\sin\theta} p_{zh}\,\sin\theta p_{zh}\Bigg), \end{aligned} \tag{16}$$

where constants α and β are two real parameters, and when $\alpha = \beta = 1/2$, it reduces to Eq. (14). For a particle moving on an arbitrary dimensional sphere one can find the similar result.

Before enclosing this short note, we can make a general ansatz that, if one insists on matching the correct quantum kinetic energy of a constraint system in Cartesian coordinates with use of the hermitian form of Cartesian momentum p_{ih}, he could start from the quantum kinetic energy of the following form:

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

where $f_i(x, y, z)$ are dummy factors in classical mechanics and can be carried out in quantum mechanics. For a particle moving on the surface of an ellipsoid, similar results exist, which is left to the readers as an exercise.

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