ROTATIONS IN 3-D CLASSICAL AND QUANTUM ROTATIONS COMPARED

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.5.6.

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

This is an example of how risky it can be to attempt to derive quantum behaviour by using logic based on classical mechanics. In classical mechanics, if we have a system with some total angular momentum with magnitude $|\mathbf{J}|$ and rotate this sytem through any angle, the magnitude of the angular momentum remains the same (although, of course, its direction changes). Based on this fact, we might think that if we start with a quantum state such as $|jm\rangle$ (where j is the total angular momentum number and m is the number for J_z), we should be able to obtain the other states with the same total angular momentum number j by rotating this state through various angles about the appropriate rotation axis. To see that this won't work, suppose we consider a state with $j=1$ and $m=1$, that is $|jm\rangle=|11\rangle$. Classically, such a system has its angular momentum aligned along the z axis, so we might think that if we rotate this system by $\frac{\pi}{2}$ about, say, the x axis, we should get a state with $m=0$, since the angular momentum is now aligned along the $-y$ axis.

To see if this works, we can use the formula for a finite rotation for a $j=1$ state. Since j remains constant, a rotation of a state $|jm\rangle$ is given by

$$D^{(1)}[R]|jm\rangle \tag{1}$$

where

$$D^{(1)}[R]=I^{(1)}+\frac{\left(\hat{\theta}\cdot\mathbf{J}^{(1)}\right)^2}{\hbar^2}(\cos\theta-1)-\frac{i\hat{\theta}\cdot\mathbf{J}^{(1)}}{\hbar}\sin\theta \tag{2}$$

For a rotation by an angle θ about the x axis, this formula reduces to

$$D^{(1)}[R(\theta\hat{\mathbf{x}})]=I^{(1)}+\frac{\left(J_x^{(1)}\right)^2}{\hbar^2}(\cos\theta-1)-\frac{iJ_x^{(1)}}{\hbar}\sin\theta \tag{3}$$

We can copy the matrix $J_x^{(1)}$ from Shankar's equation 12.5.23:

$$J_x^{(1)} = \frac{\hbar}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \tag{4}$$

We therefore have

$$\left(J_x^{(1)}\right)^2 = \frac{\hbar^2}{2} \begin{bmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{bmatrix} \tag{5}$$

Plugging these into 3 we have

$$D^{(1)}\left[R\left(\theta\hat{\mathbf{x}}\right)\right] = \frac{1}{2} \begin{bmatrix} 1+\cos\theta & -\sqrt{2}i\sin\theta & \cos\theta-1 \\ -\sqrt{2}i\sin\theta & 2\cos\theta & -\sqrt{2}i\sin\theta \\ \cos\theta-1 & -\sqrt{2}i\sin\theta & 1+\cos\theta \end{bmatrix} \tag{6}$$

In the $|jm\rangle$ basis, the state $|11\rangle$ is represented by

$$|11\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \tag{7}$$

Thus a rotation about the x axis rotates this state into:

$$\begin{aligned} |\psi\rangle &= D^{(1)}\left[R\left(\theta\hat{\mathbf{x}}\right)\right]|11\rangle & (8) \\ &= \frac{1}{2} \begin{bmatrix} 1+\cos\theta & -\sqrt{2}i\sin\theta & \cos\theta-1 \\ -\sqrt{2}i\sin\theta & 2\cos\theta & -\sqrt{2}i\sin\theta \\ \cos\theta-1 & -\sqrt{2}i\sin\theta & 1+\cos\theta \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} & (9) \\ &= \frac{1}{2} \begin{bmatrix} 1+\cos\theta \\ -\sqrt{2}i\sin\theta \\ \cos\theta-1 \end{bmatrix} & (10) \end{aligned}$$

If rotation by some angle θ could change $|11\rangle$ into the state $|10\rangle$, this result would need to be a multiple of $\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$, so we'd need to find θ such that both of the following equations are true:

$$\begin{aligned} 1+\cos\theta &= 0 & (11) \\ \cos\theta-1 &= 0 & (12) \end{aligned}$$

This is impossible, so no rotation about the x axis can change $|11\rangle$ into the state $|10\rangle$.

However, there is still a correspondence between classical and quantum mechanics if we compare the *average* values of the components of $\mathbf{J}$. That is, we want to find $\langle\mathbf{J}\rangle$ for the state 10. To do this, we need the other two matrix components $J_y^{(1)}$ and $J_z^{(1)}$. We can get $J_y^{(1)}$ from Shankar's equation 12.5.24:

$$J_y^{(1)} = \frac{i\hbar}{\sqrt{2}} \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} \tag{13}$$

$J_z^{(1)}$ is just the diagonal matrix:

$$J_z^{(1)} = \hbar \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} \tag{14}$$

We can now calculate the averages for the state 10:

$$\left\langle J_x^{(1)}\right\rangle = \left\langle \psi \left| J_x^{(1)} \right| \psi \right\rangle \tag{15}$$

$$= \frac{\hbar}{4\sqrt{2}} \left[\begin{array}{ccc} 1+\cos\theta & \sqrt{2}i\sin\theta & \cos\theta-1 \end{array}\right] \left[\begin{array}{ccc} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{array}\right] \left[\begin{array}{c} 1+\cos\theta \\ -\sqrt{2}i\sin\theta \\ \cos\theta-1 \end{array}\right] \tag{16}$$

$$= \frac{\hbar}{4} \left[\begin{array}{ccc} i\sin\theta & \sqrt{2}\cos\theta & i\sin\theta \end{array}\right] \left[\begin{array}{c} 1+\cos\theta \\ -\sqrt{2}i\sin\theta \\ \cos\theta-1 \end{array}\right] \tag{17}$$

$$= 0 \tag{18}$$

$$\left\langle J_y^{(1)}\right\rangle = \left\langle \psi \left| J_y^{(1)} \right| \psi \right\rangle \tag{19}$$

$$= \frac{i\hbar}{4\sqrt{2}} \left[\begin{array}{ccc} 1+\cos\theta & \sqrt{2}i\sin\theta & \cos\theta-1 \end{array}\right] \left[\begin{array}{ccc} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{array}\right] \left[\begin{array}{c} 1+\cos\theta \\ -\sqrt{2}i\sin\theta \\ \cos\theta-1 \end{array}\right] \tag{20}$$

$$= \frac{\hbar}{4} \left[\begin{array}{ccc} -\sin\theta & -i\sqrt{2} & \sin\theta \end{array}\right] \left[\begin{array}{c} 1+\cos\theta \\ -\sqrt{2}i\sin\theta \\ \cos\theta-1 \end{array}\right] \tag{21}$$

$$= -\hbar\sin\theta \tag{22}$$

$$\left\langle J_z^{(1)}\right\rangle = \left\langle \psi \left| J_z^{(1)} \right| \psi \right\rangle \tag{23}$$

$$= \frac{\hbar}{4} \left[\begin{array}{ccc} 1+\cos\theta & \sqrt{2}i\sin\theta & \cos\theta-1 \end{array}\right] \left[\begin{array}{ccc} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{array}\right] \left[\begin{array}{c} 1+\cos\theta \\ -\sqrt{2}i\sin\theta \\ \cos\theta-1 \end{array}\right] \tag{24}$$

$$= \frac{\hbar}{4} \left[\begin{array}{ccc} 1+\cos\theta & 0 & 1-\cos\theta \end{array}\right] \left[\begin{array}{c} 1+\cos\theta \\ -\sqrt{2}i\sin\theta \\ \cos\theta-1 \end{array}\right] \tag{25}$$

$$= \hbar\cos\theta \tag{26}$$

Thus for the average, we have

$$\langle \mathbf{J}\rangle = -\hbar\sin\theta\hat{\mathbf{y}} + \hbar\cos\theta\hat{\mathbf{z}} \tag{27}$$

In this case, a rotation by $\theta = \frac{\pi}{2}$ does indeed rotate $\langle \mathbf{J}\rangle$ so that it points along the $-y$ axis, just as it would in classical mechanics.

PINGBACKS

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