Theoretical Physics 2019/20 — Problem QT2.6

While perhaps not particularly exciting in respect to the calculations involved, this problem establishes a result of fundamental importance in Quantum Mechanics: the relation between rotations in 3D space and angular momentum operators. The key result is obtained in Part (b)(ii).

Consider a hydrogen atom in a state described by a wave function $\psi(x, y, z)$, ignoring spin and other relativistic effects. Imagine that you rotate this atom or molecule by an angle θ about the x-axis of the system of coordinates, without otherwise disturbing it in any way. For simplicity, assume that the origin of the system of coordinates is at the centre of mass, so that rotations about the x-, y- or z-axis may change the orientation of the atom but not its location in 3D space. For example, if the atom was originally in a state oriented in the z-direction (e.g., the $2\mathrm{p}_{m=0}$ state), after rotation it will be in a state oriented in a different direction but otherwise identical to the original state. The rotation thus transforms the wave function $\psi(x, y, z)$ into a new wave function $\psi'(x, y, z)$, and generally $\psi'(x, y, z)$ will not be the same function as $\psi(x, y, z)$.

Formally, the relation between the two can be expressed by the equation $|\psi'\rangle = \hat{R}_x(\theta)|\psi\rangle$, where $\hat{R}_x(\theta)$ is an operator corresponding to a rotation by an angle θ about the x-axis. Suppose that we would rotate the atom by an angle θ_1 about the x-axis and then by an angle θ_2 about the y-axis. Correspondingly, the initial state vector $|\psi\rangle$ would be transformed into the state vector $|\psi''\rangle = \hat{R}_y(\theta_2)\hat{R}_x(\theta_1)|\psi\rangle$.

(a) First, recall that any rotation in 3D space can be described by a 3×3 matrix. For example, rotating a point by an angle θ about the z-axis changes its co-ordinates from (x, y, z) to (x', y', z'), with

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}. \tag{1}$$

Rotations about the x- or y-axes can be represented similarly. Let us denote the corresponding rotation matrices by $\mathsf{R}_x(\theta)$, $\mathsf{R}_y(\theta)$ and $\mathsf{R}_z(\theta)$:

$$\mathsf{R}_x(\theta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{pmatrix}, \quad \mathsf{R}_y(\theta) = \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix}, \quad \mathsf{R}_z(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

We are particularly interested by rotations by an infinitesimally small angle ϵ. To second order in ϵ, $\cos(\epsilon) = 1 - \epsilon^2/2$ and $\sin(\epsilon) = \epsilon$, and therefore

$$\mathsf{R}_z(\epsilon) \approx \begin{pmatrix} 1-\epsilon^2/2 & -\epsilon & 0 \\ \epsilon & 1-\epsilon^2/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{2}$$

Find the corresponding approximate expressions of $\mathsf{R}_x(\epsilon)$ and $\mathsf{R}_y(\epsilon)$.

(b) A little calculation shows that

$$\mathsf{R}_y(-\epsilon)\mathsf{R}_x(-\epsilon)\mathsf{R}_y(\epsilon)\mathsf{R}_x(\epsilon) \approx \begin{pmatrix} 1 & \epsilon^2 & 0 \\ -\epsilon^2 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \approx \mathsf{R}_z(-\epsilon^2), \tag{3}$$

neglecting terms in ϵ^3 or of higher order in ϵ. (You are not asked to do this calculation. While not difficult, it is a bit tedious and it will be described in the model solution.)

Eq. (3) says that if ϵ is infinitesimal, then a rotation by ϵ about the x-axis followed by a rotation by ϵ about the y-axis followed by a rotation by $-\epsilon$ about the x-axis followed by a rotation by $-\epsilon$ about the y-axis is the same as a rotation by $-\epsilon^2$ about the z-axis. In terms of rotation operators, we must have, correspondingly,

$$\hat{R}_y(-\epsilon)\hat{R}_x(-\epsilon)\hat{R}_y(\epsilon)\hat{R}_x(\epsilon) = \hat{R}_z(-\epsilon^2). \tag{4}$$

The rotation operators appearing in this equation must differ only infinitesimally from the identity operator $\hat{I}$ if ϵ is infinitesimally small. The usual way of stating this mathematically, for a rotation about an axis $\hat{\mathbf{n}}$, is to introduce an ϵ-independent operator $\hat{J}_n$ and write the corresponding rotation operator $\hat{R}_n(\epsilon)$ as $\hat{I} - (i/\hbar)\,\epsilon\,\hat{J}_n$, to first order in ϵ. In particular, $\hat{R}_x(\pm\epsilon) \approx \hat{I} \mp (i/\hbar)\,\epsilon\,\hat{J}_x$, $\hat{R}_y(\pm\epsilon) \approx \hat{I} \mp (i/\hbar)\,\epsilon\,\hat{J}_y$ and $\hat{R}_z(-\epsilon^2) \approx \hat{I} + (i/\hbar)\,\epsilon^2\,\hat{J}_z$.

(i) Show that the operator $\hat{J}_n$ has the physical dimensions of an angular momentum.

(ii) Assume that, to second order in ϵ,

$$\hat{R}_n(\epsilon) \approx \hat{I} - \frac{i}{\hbar}\,\epsilon\,\hat{J}_n - \frac{1}{2\hbar^2}\,\epsilon^2\,\hat{J}_n^2.$$

Using this result, show that Eq. (4) implies that $[\hat{J}_x, \hat{J}_y] = i\hbar\hat{J}_z$. I.e., show that the operators $\hat{J}_x$ and $\hat{J}_y$ satisfy the same commutation relation as the orbital angular momentum operators $\hat{L}_x$ and $\hat{L}_y$ introduced in Term 1.

(c) (This part of the homework is proposed as a challenge question. It does not carry marks.) A rotation by an angle ϵ about the z-axis changes the wave function $\psi(x,y,z)$ into a wave function $\psi'(x,y,z)$ related to $\psi(x,y,z)$ through the equation

$$\psi'(x,y,z) = (1 - i\epsilon J_z/\hbar)\psi(x,y,z),$$

where J_z is the corresponding angular momentum operator in position representation. (This $\psi'(x,y,z)$ is not the same as the $\psi'(x,y,z)$ mentioned in the introduction of the problem; here the rotation is about the z-axis, not about the x-axis.) Now, rotating both the state and the co-ordinates amounts to no change; hence $\psi'(x,y,z) = \psi(x'',y'',z'')$ if (x'',y'',z'') are the initial co-ordinates of the point brought to the point of co-ordinates (x,y,z) by the rotation. For a rotation by an angle θ (here equal to ϵ), these two sets of co-ordinates are related to each other by Eq. (1):

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x'' \\ y'' \\ z'' \end{pmatrix}.$$

Deduce from this that

$$J_z = -i\hbar\left(x\,\frac{\partial}{\partial y} - y\,\frac{\partial}{\partial x}\right),$$

which is the z-component of the orbital angular momentum operator L_z. [Hint: $\mathsf{R}_z(-\theta)$ is the inverse of $\mathsf{R}_z(\theta)$.]