Physics 137B Homework 1

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Q1. Rotations about the z-axis:

(a) Let $\hat{R}_z(\delta)$ be the operator that rotates a function about the z-axis by an angle δ . It is defined by

$$\hat{R}_z(\delta)\psi(r,\theta,\phi) = \psi'(r,\theta,\phi) = \psi(r,\theta,\phi-\delta) \quad (1)$$

For an infinitessimal value of δ , show that

$$\hat{R}_z(\delta) \approx 1 - \frac{i\delta}{\hbar} \hat{L}_z$$

where \hat{L}_z is the angular momentum operator about the z-axis.

(b) Using the taylor expansion for the right hand side of Equation (1), show that in general the operator $\hat{R}_z(\delta)$ is given by

$$\hat{R}_z(\delta) = \exp\left[-\frac{i\delta}{\hbar}\hat{L}_z\right]$$

(c) Consider a small value of δ , and evaluate the action of $\hat{R}_z(\delta)$ on the position 3D vector

$$\vec{r} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

Draw a picture depicting this transformation and reconcile it with your result for $\hat{R}_z(\delta)\vec{r}$.

(d) We can readily write down the rotation operator for spin-1/2 particles, by replacing \hat{L}_z with $\hat{S}_z = \frac{\hbar}{2} \sigma_z$ where

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

is the Pauli matrix. With this, we find the rotation operator for a spin-1/2 particle to be

$$\hat{R}_{z,1/2}(\delta) = \exp\left[-\frac{i\delta}{2}\sigma_z\right]$$

Using the Taylor series of this operator and the fact $\sigma_z^2 = 1$, write $\hat{R}_{z,1/2}(\delta)$ explicitly as a two by two matrix. [Note: although you are using the Taylor series to arrive at your final expression, the final result should hold for any real value of δ]

- (e) Let $\chi_+^(z)$ be an eigenvector of σ_z with eigenvalue +1. That is, $\sigma_z \chi_+^{(z)} = \chi_+^{(z)}$. Evaluate $\hat{R}_z(\delta)\chi_+^{(z)}$. Explain your result.
- (f) Find the normalized eigenvectors $(\chi_{\pm}^{(z)})$ with eigenvalues \pm of the σ_y Pauli matrix

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

(g) Evaluate the action of the matrix you got above on the $\chi_+^{(y)}$, i.e. $\hat{R}_z(\delta)(\chi_+^{(y)})$. Explain your result.

Solutions:

(a) We define $\hat{R}_z(\delta)$ as

$$\hat{R}_z(\delta)\psi(r,\theta,\phi) = \psi(r,\theta,\phi-\delta)$$

Taylor expanding in terms of ϕ , we have

$$\psi(r,\theta,\phi-\delta) = \psi(r,\theta,\phi) - \delta \frac{\partial \psi}{\partial \phi} + \cdots$$

and the Angular Momentum operator about the z-axis can be expressed as

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial \phi}$$

$$\implies \frac{\partial}{\partial \phi} = \frac{i\hat{L}_z}{\hbar}$$

Thus,

$$\psi(r,\theta,\phi-\delta) = \psi(r,\theta,\phi) - \frac{i\delta\hat{L}_z}{\hbar}\psi(r,\theta,\phi) + \cdots$$

That is, to first order approximation, we have

$$\hat{R}_z(\theta)\psi(r,\theta,\phi) = 1 - \frac{i\delta\hat{L}_z}{\hbar}\psi(r,\theta,\phi)$$

(b) Using the Taylor expansion

$$\psi(r,\theta,\phi-\delta) = \psi - \delta \frac{\partial \psi}{\partial \phi} + \frac{1}{2!} \frac{\partial^2 \psi}{\partial \phi^2} \delta^2 + \cdots$$

$$\implies \hat{R}_z(\delta)\psi(r,\theta,\phi) = \left(\mathbf{1} - \delta \frac{\partial}{\partial \phi} + \frac{1}{2!} \frac{\partial^2}{\partial \phi^2} \delta^2 + \cdots\right) \psi(r,\theta,\phi)$$

$$\implies \hat{R}_z(\delta)\psi(r,\theta,\phi) = \left(\mathbf{1} - \frac{i\delta}{\hbar} \hat{L}_z + \cdots\right) \psi(r,\theta,\phi)$$

$$\implies \hat{R}_z(\delta) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{i\delta}{\hbar} \hat{L}_z\right)^n$$

Therefore,

$$\hat{R}_z(\delta) = \exp\left[-\frac{i\delta}{\hbar}\hat{L}_z\right]$$

(c) We consider an arbitrary 3D position vector

$$\vec{r} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} r \sin(\theta) \cos(\phi) \\ r \sin(\theta) \sin(\phi) \\ r \cos(\theta) \end{pmatrix}$$

Now, acting on this vector with $\hat{R}_z(\delta)$ has the effect of carrying out the transformation $\phi \to \phi - \delta$, so

$$\vec{r}' = \begin{pmatrix} r\sin(\theta)\cos(\phi - \delta) \\ r\sin(\theta)\sin(\phi - \delta) \\ r\cos(\theta) \end{pmatrix}$$
$$= \begin{pmatrix} r\sin(\theta)\left[\cos(\phi)\cos(\delta) + \sin(\phi)\sin(\delta)\right] \\ r\sin(\theta)\left[\sin(\phi)\cos(\delta) - \cos(\phi)\sin(\delta)\right] \\ r\cos(\theta) \end{pmatrix}$$

Since δ is small, $\cos(\delta) \approx 1$ and $\sin(\delta) \approx \delta$. So,

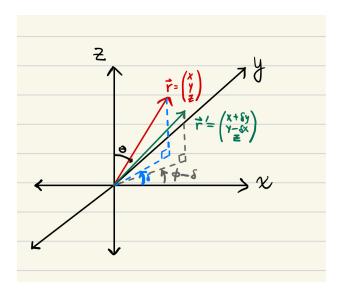
$$\vec{r}' = \begin{pmatrix} r\sin(\theta)[\cos(\phi) \cdot 1 + \sin(\phi) \cdot \delta] \\ r\sin(\theta)[\sin(\phi) \cdot 1 - \cos(\phi) \cdot \delta] \\ r\cos(\theta) \end{pmatrix}$$

$$= \begin{pmatrix} r\sin(\theta)\cos(\phi) + \delta \cdot r\sin(\theta)\cos(\phi) \\ r\sin(\theta)\sin(\phi) - \delta \cdot r\sin(\theta)\cos(\phi) \\ r\cos(\theta) \end{pmatrix}$$

$$= \begin{pmatrix} x + \delta y \\ y - \delta x \\ z \end{pmatrix}$$

Thus, applying the $\hat{R}_z(\delta)$ operator with a small value of δ has the effect of the transformation:

$$\begin{array}{ccc} x & & x + \delta y \\ y & \rightarrow & y - \delta x \\ z & & z \end{array}$$



(d) For a spin-1/2 particle, we have

$$\hat{R}_{z,1/2}(\delta) = \exp\left[-\frac{i\delta}{2}\sigma_z\right]$$

We now want to explicitly find the matrix representation of this operator, using the taylor series and the fact that $\sigma_z^2 = 1$.

Now,

$$\begin{split} \hat{R}_{z,1/2}(\delta) &= \exp\left[-\frac{i\delta}{2}\sigma_z\right] \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} \cdot \left(-\frac{i\delta}{2}\sigma_z\right)^n \end{split}$$

and

$$\sigma_z^2 = 1 \implies \sigma_z^{2k} = 1$$
 $\sigma_z^2 = 1 \implies \sigma_z^{2k+1} = \sigma_z$

So,

$$\begin{split} \hat{R}_{z,1/2}(\delta) &= \sum_{k \in \mathbb{N}} \left[\frac{1}{(2k)!} \left(-\frac{i\delta}{2} \right)^{2k} \mathbb{1} \right] + \sum_{k \in \mathbb{N}} \left[\frac{1}{(2k+1)!} \left(-\frac{i\delta}{2} \right)^{2k+1} \sigma_z \right] \\ &= \left[\sum_{k \in \mathbb{N}} \frac{1}{(2k)!} \left(-\frac{i\delta}{2} \right)^{2k} \right] \mathbb{1} + \left[\sum_{k \in \mathbb{N}} \frac{1}{(2k+1)!} \left(-\frac{i\delta}{2} \right)^{2k+1} \right] \sigma_z \end{split}$$

For the sake of convenience, let's denote the two sums as

$$A \equiv \sum_{k \in \mathbb{N}} \frac{1}{(2k)!} \left(-\frac{i\delta}{2} \right)^{2k}$$
$$B \equiv \sum_{k \in \mathbb{N}} \frac{1}{(2k+1)!} \left(-\frac{i\delta}{2} \right)^{2k+1}$$

Recall that the matrix representations of $\mathbbm{1}$ and σ_z are

$$1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Then,

$$\begin{split} \hat{R}_{z,1/2}(\delta) &= A\mathbb{1} + B\sigma_z \\ &= \begin{pmatrix} A & 0 \\ 0 & A \end{pmatrix} + \begin{pmatrix} B & 0 \\ 0 & -B \end{pmatrix} \\ &= \begin{pmatrix} A + B & 0 \\ 0 & A - B \end{pmatrix} \end{split}$$

But notice that

$$A + B = \sum_{k \in \mathbb{N}}^{\infty} \frac{1}{k!} \left(-\frac{i\delta}{2} \right)^k$$
$$= e^{-\frac{i\delta}{2}}$$

and

$$A - B = \sum_{k \in \mathbb{N}}^{\infty} \frac{1}{k!} \cdot (-1)^k \left(-\frac{i\delta}{2} \right)^k$$
$$= \sum_{k \in \mathbb{N}}^{\infty} \frac{1}{k!} \cdot \left(-1 \times -\frac{i\delta}{2} \right)^k$$
$$= \sum_{k \in \mathbb{N}}^{\infty} \frac{1}{k!} \left(\frac{i\delta}{2} \right)^k$$
$$= e^{+\frac{i\delta}{2}}$$

Therefore, the final expression we get for the rotation operator is

$$\hat{R}_z(\delta) = \begin{pmatrix} e^{-\frac{i\delta}{2}} & 0\\ 0 & e^{+\frac{i\delta}{2}} \end{pmatrix}$$

(e) We let $\chi_+^{(z)}$ be the eigenvector of σ_z having eigenvalue +1 i.e. $\sigma_z \chi_+^{(z)} = \chi_+^{(z)}$.

$$\sigma_z \chi_+^{(z)} = \chi_+^{(z)}$$

$$\implies \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} a \\ b \end{pmatrix}$$

$$\implies \begin{cases} a = a \\ b = -b \end{cases}$$

So, b = 0 and a can be any real number (before normalization), but as per convention let's choose a = 1. So,

$$\chi_{+}^{(z)} = \begin{pmatrix} 1\\0 \end{pmatrix}$$

Applying the rotation operator then gives us

$$\hat{R}_{z}(\delta)\chi_{+}^{(z)} = \begin{pmatrix} e^{-i\delta/2} & 0\\ 0 & e^{+i\delta/2} \end{pmatrix} \begin{pmatrix} 1\\ 0 \end{pmatrix}$$
$$= \begin{pmatrix} e^{-i\delta/2}\\ 0 \end{pmatrix}$$
$$= e^{-i\delta/2} \begin{pmatrix} 1\\ 0 \end{pmatrix}$$

Thus.

$$\hat{R}_{z,1/2}(\delta)\chi_{+}^{(z)} = e^{-i\delta/2}\chi_{+}^{(z)}$$

So, applying the rotation matrix does not change the physical system, which makes sense.

$$\sigma_z \left(\hat{R}_{z,1/2}(\delta) \chi_+^{(z)} \right) = \sigma_z \left(e^{-i\delta/2} \chi_+^{(z)} \right)$$

$$= e^{-i\delta/2} \left(\sigma_z \chi_+^{(z)} \right)$$

$$= e^{-i\delta/2} \chi_+^{(z)}$$

$$= \hat{R}_{z,1/2}(\delta) \chi_+^{(z)}$$

So, the rotated spinor is also an eigenspinor of σ_z with eigenvalue +1. Intuitively this makes sense, because $\chi_+^{(z)}$ was already completely "aligned" with the z-axis, so rotation about the z-axis should make no observable difference.

(f) We want to find the normalized eigenvectors $(\chi_{\pm}^{(y)})$ with eigenvalue ± 1 of the σ_y Pauli Matrix,

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$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

Let $\chi = \begin{pmatrix} a \\ b \end{pmatrix}$ be an eigenvector of σ_y with eigenvalue ± 1 . Then,

$$\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \pm \begin{pmatrix} a \\ b \end{pmatrix}$$

$$\implies \begin{pmatrix} -ib \\ ia \end{pmatrix} = \pm \begin{pmatrix} a \\ b \end{pmatrix}$$

For the +1 case:

$$-ib = a$$
$$ia = b$$

$$\implies -i(ia) = a$$
$$\implies \boxed{a = a}$$

and

$$b = -\frac{1}{i}a$$

$$\Longrightarrow b = ia$$

i.e we can arbitrarily choose a, get b from b=ia, and then normalize the spinor as $\chi^\dagger\chi=1$. We found that the (+1)-eigenspinor has the form $\chi_+^{(y)}=\binom{a}{ia}$.

$$(\chi_{+}^{(y)})^{\dagger}\chi_{+}^{(y)} = 1$$

$$\implies (a -ia) \binom{a}{ia} = 1$$

$$\implies a^2 + a^2 = 1$$

$$\implies a^2 = \frac{1}{2}$$

$$\implies a = \frac{1}{\sqrt{2}}$$

So, the +1 eigenspinor is

$$\chi_{+}^{(y)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\i \end{pmatrix}$$

For the -1 case:

$$-ib = -a$$
$$ia = -b$$

$$\implies i(-ia) = a$$
$$\implies \boxed{a = a}$$

and

$$b = -ia$$

So, following the same argument as before, $(\chi_{-}^{(y)})^{\dagger}\chi_{-}^{(y)}=1$ gives

$$(a \quad ia) \begin{pmatrix} a \\ -ia \end{pmatrix} = 1$$

$$\implies a^2 + a^2 = 1$$

$$\implies \boxed{a = \frac{1}{\sqrt{2}}}$$

So, the (-1)-eigenspinor is

$$\chi_{-}^{(y)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\ -i \end{pmatrix}$$

To summarise, the normalized eigenspinors of the σ_z Pauli matrix are $\chi_+^{(y)}$ and $\chi_-^{(y)}$ given by

$$\chi_{+}^{(y)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\i \end{pmatrix}$$
$$\chi_{+}^{(y)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\-i \end{pmatrix}$$

(g) Now, let's evaluate the rotation matrix on $\chi_{+}^{(y)}$.

$$\hat{R}_z(\delta)\chi_+^{(y)} = \begin{pmatrix} e^{-i\delta/2} & 0\\ 0 & e^{+i\delta/2} \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\ i \end{pmatrix}$$
$$= \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\delta/2} \cdot 1 + 0 \cdot i\\ 0 \cdot 1 + e^{+i\delta/2} \cdot i \end{pmatrix}$$
$$= \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\delta/2}\\ i e^{+i\delta/2} \end{pmatrix}$$

Is this rotated spinor still an eigenspinor of σ_y ?

$$\begin{split} \sigma_y \left(\hat{R}_z(\delta) \chi_+^{(y)} \right) &= \sigma_y \left(\frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\delta/2} \\ i e^{+i\delta/2} \end{pmatrix} \right) \\ &= \frac{1}{\sqrt{2}} \sigma_y \begin{pmatrix} e^{-i\delta/2} \\ i e^{+i\delta/2} \end{pmatrix} \\ &= \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} e^{-i\delta/2} \\ i e^{+i\delta/2} \end{pmatrix} \\ &= \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \cdot e^{-i\delta/2} - i \cdot i e^{+i\delta/2} \\ i e^{-i\delta/2} + 0 \cdot e^{+i\delta/2} \end{pmatrix} \\ &= \frac{1}{\sqrt{2}} \begin{pmatrix} e^{+i\delta/2} \\ i e^{-i\delta/2} \end{pmatrix} \\ &= \frac{1}{\sqrt{2}} e^{+i\delta} \begin{pmatrix} e^{-i\delta/2} \\ i e^{-3i\delta/2} \end{pmatrix} \end{split}$$

So, $(\hat{R}_z(\delta)\chi^{+(y)})$ is not an eigenspinor of σ_y . Intuivitely, this makes sense since rotating the eigenspinor $\chi_+^{(y)}$ (which was originally "completely oriented in the y-direction" in some sense) about the z-axis would seem to introduce some x-axis alignment.

Q2. Unitary Operators: We have now seen two examples of continuous unitary transformations that are of the form $\hat{U}(\delta) = \exp(-\hat{M}\delta)$ where \hat{M} is hermitian. Prove that any operator of this form is unitary as long as \hat{M} is hermitian.

Proof: Let \hat{M} be a Hermitian operator i.e. $\hat{M} = \hat{M}^{\dagger}$, and consider the operator

$$\hat{U}(\delta) = \exp(-i\hat{M}\delta)$$

We want to show that \hat{U} is unitary i.e.

$$\hat{U}(\delta)^{\dagger}\hat{U}(\delta) = \mathbb{1}$$

What is \hat{U}^{\dagger} ?

$$\begin{split} \hat{U}^{\dagger} &= \exp(-i\hat{M}\delta) \\ &= \left[\sum_{n=0}^{\infty} \frac{1}{n!} \left(-i\hat{M}\delta\right)^{n}\right]^{\dagger} \\ &= \sum_{n=0}^{\infty} \left[\frac{1}{n!} \left(-i\hat{M}\delta\right)^{n}\right]^{\dagger} \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} \delta^{n} \left[(-i\hat{M})^{n}\right]^{\dagger} \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} \delta^{n} (\hat{M}^{n})^{\dagger} \left[(-i)^{n}\right]^{\dagger} \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} \delta^{n} \hat{M}^{n} \left[(-i)^{n}\right]^{\dagger} \end{split}$$

Let's break into cases and see what $[(-i)^n]^{\dagger} = [(-1)^n (i)^n]^{\dagger}$ evaluates to in each case.

For $n = 4k + 0, k \in \mathbb{Z}$:

$$(-1)^n \cdot i^n = 1 \cdot 1$$

$$\implies [(-i)^n]^{\dagger} = 1^{\dagger} = 1$$

For $n = 4k + 1, k \in \mathbb{Z}$:

$$(-1)^n \cdot i^n = -1 \cdot i$$

$$\implies [(-i)^n]^{\dagger} = (-i)^{\dagger} = i$$

For $n = 4k + 2, k \in \mathbb{Z}$:

$$(-1)^n \cdot i^n = 1 \cdot (-1)$$

$$\implies [(-i)^n]^{\dagger} = (-1)^{\dagger} = -1$$

For $n = 4k + 3, k \in \mathbb{Z}$:

$$(-1)^n \cdot i^n = (-1) \cdot (-i)$$

$$\implies [(-i)^n]^{\dagger} = i^{\dagger} = -i$$

We notice that these coincide exactly with the powers of i, so

$$\hat{U}^{\dagger} = \sum_{n=0}^{\infty} \frac{1}{n!} \delta^n \hat{M}^n i^n$$
$$= \sum_{n=0}^{\infty} \frac{1}{n!} \left(i \hat{M} \delta \right)^n$$
$$= \exp\left(+ i \hat{M} \delta \right)$$

So, if $\hat{U} = \exp(-i\hat{M}\delta)$ then $\hat{U}^{\dagger} = \exp(+i\hat{M}\delta)$.

To show that $\hat{U}^{\dagger}\hat{U} = 1$, we use the following well-known identity:

For linear operators \hat{A} and \hat{B} ,

$$e^{\hat{A}}\hat{B}e^{-\hat{A}} = \mathbb{1} + [\hat{A}, \hat{B}] + \frac{1}{2!}[\hat{A}, [\hat{A}, \hat{B}]] + \cdots$$

Proof Sketch: Through some brute force, we can show

$$\begin{split} e^{\hat{A}}\hat{B}e^{-\hat{A}} &= \left(\mathbbm{1} + \hat{A} + \frac{1}{2!}\hat{A}^2 + \frac{1}{3!}\hat{A}^3 + \cdots\right)\hat{B}\left(\mathbbm{1} - \hat{A} + \frac{1}{2!}\hat{A}^2 - \frac{1}{3!}\hat{A}^3 + \cdots\right) \\ &= \mathbbm{1} + \left(\hat{A}\hat{B} - \hat{B}\hat{A}\right) + \frac{1}{2!}\hat{A}^2\hat{B} - \hat{A}\hat{B}\hat{A} + \frac{1}{2!}\hat{B}\hat{A}^2 + \cdots \\ &= \mathbbm{1} + \left(\hat{A}\hat{B} - \hat{B}\hat{A}\right) + \frac{1}{2!}[\hat{A}, [\hat{A}, \hat{B}]] - \frac{1}{2!}[\hat{A}, \hat{B}]\hat{A} + \cdots \\ &\implies e^{\hat{A}}\hat{B}e^{-\hat{A}} = \mathbbm{1} + [\hat{A}, \hat{B}] + \frac{1}{2!}[\hat{A}, [\hat{A}, \hat{B}]] + \frac{1}{3!}[\hat{A}, [\hat{A}, [\hat{A}, \hat{B}]]] + \cdots \end{split}$$

So, applying this formula with $\hat{A} = i\hat{M}\delta$ and $\hat{B} = 1$ we get

$$e^{i\hat{M}\delta}\mathbbm{1} e^{-i\hat{M}\delta}=\mathbbm{1}+[e^{i\hat{M}\delta},\mathbbm{1}]+\frac{1}{2!}[e^{i\hat{M}\delta},[e^{i\hat{M}\delta},\mathbbm{1}]]+\cdots$$

Now, the identity operator 1 commutes with every linear operator, so the only non-vanishing term on the RHS is the first term i.e. 1 itself.

Therefore,

$$e^{i\hat{M}\delta}e^{-i\hat{M}\delta} = \mathbb{1}$$

$$\Longrightarrow \hat{U}^{\dagger}\hat{U} = \mathbb{1}$$

We can also show $\hat{U}\hat{U}^{\dagger}$ in exactly the same way. So, U is unitary.

Q3. Conservation Laws: For each of the Hamiltonians below, determine which of the following are conserved quantities:

$$\{p_x, p_y, p_z, p^2, S_x, S_y, S_z, L_x, L_y, L_z, L^2\}$$

where p_j, S_j, L_j are the expectation values of the momentum, spin, and orbital angular momentum along the j^{th} direction.

- (a) The Hamiltonian of a Free Electron: $\hat{H} = \frac{\hat{p}^2}{2m}$, where $\hat{p}^2 = \hat{p_x}^2 + \hat{p_y}^2 + \hat{p_z}^2$.
- (b) Hamiltonian of an electron in the presence of a constant background electric field pointing along the z- axis: $\hat{H}_E=\frac{\hat{p}}{2m}+eE_0\hat{z}$, where E is the value of the electric field intensity.
- (c) Hamiltonian of an electron in the presence of a weak constant magnetic field (B_z) along the z-axis: $\hat{H}_E = \frac{\hat{p}}{2m} + B_z \left(e\frac{\hat{L}_z}{2m} \gamma \hat{S}_z\right)$, where γ is the gyromagnetic ratio of the electron, i.e. it is constant.

We know that for an operator \hat{Q} , the expectation value $\langle \hat{Q} \rangle$ is a conserved quantity if \hat{Q} commutes with the Hamiltonian i.e. $[\hat{H}, \hat{Q}] = 0$.

The Angular Momentum operator in the i^{th} direction is

$$\hat{L}_i = \epsilon_{ijk} \hat{X}_i \hat{P}_k$$

where we are using the Einstein Summation Convention, rather than explicitly writing the summations out.

Now, starting from the canonical commutation relations

$$[\hat{X}_i, \hat{X}_j] = 0 = [\hat{P}_i, \hat{P}_j]; \quad [\hat{X}_i, \hat{P}_j] = i\hbar \delta_{ij};$$

we can obtain some useful relations:

1. Between \hat{L}_i and \hat{X}_l :

$$\begin{split} [\hat{L}_i, \hat{X}_l] &= [\epsilon_{ijk} \hat{X}_l \hat{P}_k, X_l] \\ &= \epsilon_{ijk} [X_j P_k, X_l] \\ &= \epsilon_{ijk} \left([X_j, X_l] P_k + X_j [P_k, X_l] \right) \\ &= \epsilon_{ijk} \left(0 \cdot P_k + X_j (-i\hbar \delta_{lk}) \right) \\ &= -i\hbar \epsilon_{ijk} X_j \delta_{lk} \\ &= -i\hbar \epsilon_{ijl} X_j \\ \Longrightarrow \left[\hat{L}_i, \hat{X}_l \right] &= i\hbar \epsilon_{ilj} X_j \end{split}$$

2. Between \hat{L}_i and \hat{P}_l :

$$\begin{split} [\hat{L}_i, \hat{P}_l] &= [\epsilon_{ijk} X_j P_k, P_l] \\ &= \epsilon_{ijk} [X_j P_k, P_l] \\ &= \epsilon_{ijk} \left([X_j, P_l] P_k + X_j [P_k, P_l] \right) \\ &= \epsilon_{ijk} \left(i\hbar \delta_{jl} P_k + X_j \cdot 0 \right) \\ &= i\hbar \epsilon_{ilk} P_k \end{split}$$

$$\hat{L}_i, \hat{P}_l = i\hbar\epsilon_{ilk}P_k$$

3. Between \hat{L}_i and \hat{L}_j :

$$\begin{split} [L_i,L_j] &= [\epsilon_{iab}\hat{X}_a\hat{P}_b,\epsilon_{jmn}\hat{X}_m\hat{P}_n] \\ &= \epsilon_{iab}\epsilon_{jmn}[\hat{X}_a\hat{P}_b,\hat{X}_m\hat{P}_n] \\ &= \epsilon_{iab}\epsilon_{jmn}\left([\hat{X}_a\hat{P}_b,\hat{X}_m]\hat{P}_n + \hat{X}_m[\hat{X}_a\hat{P}_b,\hat{P}_n]\right) \\ &= \epsilon_{iab}\epsilon_{jmn}\left([\hat{X}_a\hat{P}_b,\hat{X}_m]\hat{P}_n + \hat{X}_m[\hat{X}_a\hat{P}_b,\hat{P}_n]\right) \\ &= \epsilon_{iab}\epsilon_{jmn}\left([\hat{X}_a\hat{P}_b,\hat{X}_m]\hat{P}_n + \hat{X}_a[\hat{P}_b,\hat{X}_m]\hat{P}_n + \hat{X}_m[\hat{X}_a,\hat{P}_n]\hat{P}_b + \hat{X}_m\hat{X}_a[\hat{P}_b,\hat{P}_n]\right) \\ &= \epsilon_{iab}\epsilon_{jmn}\left(\hat{X}_a[\hat{P}_b,\hat{X}_m]\hat{P}_n + \hat{X}_m[\hat{X}_a,\hat{P}_n]\hat{P}_b\right) \\ &= \epsilon_{iab}\epsilon_{jmn}\left(\hat{X}_a(-i\hbar\delta_{bm})\hat{P}_n + \hat{X}_m(i\hbar\delta_{an})\hat{P}_b\right) \\ &= -i\hbar\epsilon_{iab}\epsilon_{jnb}\hat{X}_a\hat{P}_n + i\hbar\epsilon_{iab}\epsilon_{jma}\hat{X}_m\hat{P}_b \\ &= i\hbar\epsilon_{iab}\epsilon_{jnb}\hat{X}_a\hat{P}_n - i\hbar\epsilon_{iba}\epsilon_{jma}\hat{X}_m\hat{P}_b \end{split}$$

Using the well known identity for the product of two levi-civita symbols, we can express $\epsilon_{iab}\epsilon_{jbn}$ as

$$\epsilon_{iab}\epsilon_{jbn} = \delta_{ij}\delta_{an} - \delta_{in}\delta_{aj}$$

and $\epsilon_{iab}\epsilon_{jma}$ as

$$\epsilon_{iab}\epsilon_{ima} = \delta_{ij}\delta_{bm} - \delta_{im}\delta_{bj}$$

So,

$$\begin{split} [\hat{L}_i,\hat{L}_j] &= i\hbar(\delta_{ij}\delta_{an} - \delta_{in}\delta_{aj})\hat{X}_a\hat{P}_n - i\hbar(\delta_{ij}\delta_{bm} - \delta_{im}\delta_{bj})\hat{X}_m\hat{P}_b \\ &= \underline{i}\hbar\delta_{ij}\hat{X}_a\hat{P}_a - i\hat{X}_j\hat{P}_i - i\hbar\hat{X}_b\hat{P}_b + i\hbar\hat{X}_i\hat{P}_j \\ &= i\hbar\left(\hat{X}_i\hat{P}_i - \hat{X}_j\hat{P}_i\right) \\ &= i\hbar\epsilon_{ijk}\hat{L}_k \end{split}$$

Thus,

$$\boxed{[L_i, L_k] = i\hbar\epsilon_{ijk}\hat{L}_k}$$

Also, the Spin Operators follow exactly the same algebra as the Orbital Angular Momentum Operators i.e.

$$[\hat{S}_i, \hat{S}_k] = i\hbar\epsilon_{ijk}\hat{S}_k$$

However, for an electron, spin is an internal degree of freedom and is completely independent of the particle's position or momentum.

We can describe the Hilbert space of the Electron V_e , as being a tensor product of an infinitedimensional hilbert space V_o describing its orbital degrees of freedom and a two-dimensional space V_s describing its spin degrees of freedom:

$$\mathbb{V}_e = \mathbb{V}_o \otimes \mathbb{V}_s$$

Thus, the Spin operators \hat{S}_i (which act on \mathbb{V}_s) act on a different hilbert space than the position and momentum operators (which act on \mathbb{V}_o), and thus commute with them in all directions:

$$\hat{\hat{S}_i, \hat{X}_j} = 0$$
$$\hat{\hat{S}_i, \hat{P}_j} = 0$$

for all i, j. As a result, the expected values associated with the spin operators are always conserved.

Now that we have all of our basic commutation relations in hand, lets tackle each Hamiltonian:

(a) Free Electron:

$$\hat{H} = \frac{\hat{P}^2}{2m}$$

• Since the Hamiltonian only has the momentum squared operator in it, certainly it commutes with \hat{P}^2

$$[\hat{H}, \hat{P}^2] = [\frac{\hat{P}^2}{2m}, \hat{P}^2] = \frac{1}{2m}[\hat{P}^2, \hat{P}^2] = 0$$

• Now, since $\hat{P}^2 = \hat{P}_x^2 + \hat{P}_y^2 + \hat{P}_z^2$ and $[\hat{P}_i, \hat{P}_j] = 0$ for i, j = x, y, z we immediately find that

$$[\hat{H}, \hat{P}^2] = 0 \implies [\hat{H}, \hat{P}_i^2] = 0$$

• The Hamiltonian is rotationally invariant, so \hat{H} commutes with each \hat{L}_i and with \hat{L}^2 . We can show this explicitly as

$$\begin{bmatrix}
\hat{P}^2 \\
2m
\end{bmatrix}, \hat{L}_m
\end{bmatrix} = -\frac{1}{2m} \left[\hat{L}_m, \hat{P}_i \hat{P}_i\right] \quad \text{(Using Einstein Summation Convention)}$$

$$= -\frac{1}{2m} \left([\hat{L}_m, \hat{P}_i] \hat{P}_i + \hat{P}_i [\hat{L}_m, \hat{P}_i] \right)$$

$$= -\frac{1}{2m} \left[(\epsilon_{mik} i\hbar \hat{P}_k) \hat{P}_i + \hat{P}_i (\epsilon_{mik} i\hbar \hat{P}_k) \right]$$

$$= -\frac{i\hbar}{2m} \epsilon_{mik} [\hat{P}_k, \hat{P}_i]$$

$$= 0 \quad \text{(Momentum components always commute)}$$

= 0 (Momentum components always commute)

$$\left[\hat{H},\hat{L}_m\right] = 0$$

So, the Hamiltonian commutes with each \hat{L}_m and thus also commutes with \hat{L}^2 as

$$[\hat{H}, \hat{L}^2] = [\hat{H}, \hat{L}_m \hat{L}_m]$$

$$= [\hat{H}, \hat{L}_m] \hat{L}_m + \hat{L}_m [\hat{H}, \hat{L}_m]$$

$$= 0 + 0$$

$$= 0$$

Summary: The Free Electron Hamiltonian commutes with all the operators associated with the quantities we're interested in, so all of their expectation values are conserved.

(b) Electron in Constant Electric Field:

$$\hat{H}_E = \frac{\hat{p}^2}{2m} + eE_0\hat{z}$$

which can be re-written in slightly different notation as

$$\hat{H}_E = \frac{\hat{P}^2}{2m} + eE_0\hat{X}_3$$

We know of course that the free part of the hamiltonian commutes with all the operators, so we are interested in the behavior of $eE_0\hat{X}_3$.

• We know that $[\hat{X}_i, \hat{P}_i] = i\hbar \delta_{ij}$ so

$$[eE_0\hat{X}_3, \hat{P}_j] = eE_0i\hbar\delta_{i3}$$

This means that the Hamiltonian commutes with the momentum operators <u>other than</u> $\hat{P}_3 = \hat{p}_z$.

- Since it doesn't commute with the momenta in every direction, it also doesn't commute with \hat{P}^2 .
- We know that $[\hat{X}_l, \hat{L}_i] = -i\hbar\epsilon_{ilj}X_j$. So.

$$[eE_0\hat{X}_3, \hat{L}_i] = -i\hbar\epsilon_{i3j}X_j$$

When i=3, the levi-civita tensor becomes zero for all terms, so we have $[eE_0\hat{X}_3, \hat{L}_3]=0$ i.e. the Hamiltonian commutes with the \hat{L}_z operator. However, it doesn't commute with the other directions.

• Since the Hamiltonian doesn't commute with the Angular Momentum with respect to all axes, it doesn't commute with the total angular momentum \hat{L}^2 .

Summary: The p_x , p_y , l_z and spin expected values are conserved. But the p_z , p^2 , L_x , L_y , L^2 values are not.

(c) Electron in a weak Constant Magnetic Field:

$$\hat{H}_E = \frac{\hat{P}^2}{2m} + B_z \left(e \frac{\hat{L}_z}{2m} - \gamma \hat{S}_z \right)$$

Again, we know the free part $\hat{P}^2/2m$ commutes with all of the operators, so we only discuss the other components of the Hamiltonian

- Using the commutation relations between \hat{L}_i and \hat{P}_j found earlier, we know that \hat{L}_z only commutes with \hat{P}_z . The \hat{S}_z present in the hamiltonian commutes with all momentum operators since they act on different hilbert spaces.
- Now, the spin matrices \hat{S}_x and \hat{S}_y commute with \hat{P}^2 and \hat{L}_z , but do not commute with \hat{S}_z due to the commutation relation

$$[\hat{S}_i, \hat{S}_k] = i\hbar\epsilon_{ijk}\hat{S}_k$$

The operator \hat{S}_z does commute with itself so it commutes with the hamiltonian as a whole.

• The angular momentum operators all commute with the spin operators since they act on different hilbert spaces. However, \hat{L}_x and \hat{L}_y do not commute with \hat{L}_z , so only \hat{L}_z commutes with the hamiltonian as a whole.

Summary: The conserved expected values are: p_z, s_z, l_z . All other expected values are not conserved.