1 Lecture 15 (April 30th)

Chapter 5 Essential Elements

Definition. (Quantum State) A pure quantum state is defined as a ray in a Hilbert space. Here, a Hilbert space is a complex vector space with the inner product that is a complete. Some examples of Hilbert spaces are L^2, $\boldsymbol{C}^n$, and $M_{n\times n}$

Definition. (Ray) By a ray, we mean that for $|\psi\rangle \in \mathcal{H}$, $\{c|\psi\rangle\}$ where $c \in \mathcal{C}$. As we are considering normalised wave functions, $\langle\psi|\psi\rangle = 1$ and $|c|^2\langle\psi|\psi\rangle = 1$ and $|c|^2 = 1$, leading to $c = e^{i\theta}$ and $\{e^{i\theta}\psi\}$. This is saying that a state is equivalent up to a transformation that conserves the modulus.

Definition. (Composite system) Consider two Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$. In the discussion of a system comprised of both Hilbert spaces, we necessarily look at bilinear maps. A composite system of quantum states is therefore expressed as a tensor product

$$|\psi\rangle_1 \otimes |\psi\rangle_2 \in \mathcal{H}_1 \otimes \mathcal{H}_2$$

When an element in such a tensor product can be expressed as a tensor product like the above, we say that such an element is separable. If not, we say that the element is entangled.

Example. (Kronecker product) We can consider the Kronecker product as a specific example of a tensor product. Let

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \quad B = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}$$

We can use the representation

$$A \otimes B = \begin{pmatrix} aB & bB \\ cB & dB \end{pmatrix} = \begin{pmatrix} a\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} & b\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \\ \\ c\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} & d\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \end{pmatrix}$$

Example. Now, let $A = (x, y)$ and $B = (a, b)$. Then,

$$A \otimes B = (xB, yB) = \begin{pmatrix} xa & ya \\ xb & yb \end{pmatrix}$$

Also,

$$B \otimes A = \begin{pmatrix} a(x, y) \\ b(x, y) \end{pmatrix} = \begin{pmatrix} ax & ay \\ bx & by \end{pmatrix}$$

Definition. (Observables, their adjoint, and their expectation) An operator is a linear function from a Hilbert space to the complex numbers (linear map).

$$\hat{O} : \mathcal{H} \to \boldsymbol{C}$$

An adjoint of an operator is an operator that satisfies (we often denote $\hat{O}|\psi\rangle = |\hat{O}\psi\rangle$)

$$\langle \hat{O}\phi|\psi\rangle = \langle \phi|\hat{O}^\dagger|\psi\rangle$$

where $\hat{O}^\dagger$ is the adjoint. Notice how

$$\langle \hat{O}\phi|\psi\rangle^* = \langle \psi|\hat{O}\phi\rangle = \langle \hat{O}^\dagger\psi|\phi\rangle = \langle \phi|\hat{O}^\dagger\psi\rangle^*$$

and that the definition for an adjoint operator can also be written as

$$\langle \hat{O}^\dagger\phi|\psi\rangle = \langle \phi|\hat{O}|\psi\rangle$$

Now, for the expectation value for a measurement to be real, we have

$$\langle \psi|\hat{O}|\psi\rangle = \langle \psi|\hat{O}|\psi\rangle^* = \langle \hat{O}\psi|\psi\rangle = \langle \psi|\hat{O}^\dagger|\psi\rangle$$

That is, for an expectation value for a measurement to be real, the observable must be Hermitian.

2 Lecture 16 (March 5th)

(Online lecture on partial differential equations)

3 Lecture 17 (May 7th)

Definition. (Adjointness as a suffient condition for real eigenvalues) An adjoint operator is defined as

$$\langle \psi|A^\dagger|\phi\rangle = \langle A\psi|\phi\rangle$$

Where a self-adjoint operator is an operator that satisfies

$$A = A^\dagger$$

We have previously seen how the following inner product is real if self-adjointness holds.

$$\langle \psi|A|\psi\rangle$$

Theorem. (Completeness relation) A basis is complete if and only if the completeness relation holds.

$$\mathbf{1} = \sum_n |n\rangle\langle n|$$

Proof. Suppose that a Hilbert space has a complete orthonormal basis satisfying $\langle n|m\rangle = \delta_{nm}$. For $|\psi\rangle \in \mathcal{H}$, we have the following representation.

$$|\psi\rangle = \sum_n c_n |n\rangle$$

The coefficients are given by

$$\langle m|\psi\rangle = \sum_n c_n \langle m|n\rangle = c_m \quad \text{and} \quad |\psi\rangle = \sum_n \langle n|\psi\rangle |n\rangle = \sum_n |n\rangle\langle n|\psi\rangle$$

From the above, we have

$$\mathbf{1} = \sum_n |n\rangle\langle n|$$

which is called the completeness relation. Conversely, we can assume that the above is true for any $|\psi\rangle$, and any vector could be expanded in terms of the basis. We have thus proved the theorem. $\square$

Definition. (Dual spaces and the Riesz Lemma) The dual space of a vector space V is the vector space that contains all the linear maps $T : V \to \boldsymbol{C}$ that act on V. There is a one-to-one correspondence between the dual space and the inner products $\langle \cdot |w\rangle$ and moreover the dual space and V.

$$\underbrace{\langle\psi|}_{\text{bra}} \longleftrightarrow \underbrace{|\psi\rangle}_{\text{ket}} \quad \text{and} \quad \langle\psi|A^\dagger \longleftrightarrow A|\psi\rangle$$

Notice that from $\langle\psi|\phi\rangle^* = \langle\phi|\psi\rangle$, we can deduce the conjugate linearity of the first argument. Consider how

$$\begin{aligned}
\langle\beta|c_1v_1 + c_2v_2\rangle &= c_1\langle\beta|v_1\rangle + c_2\langle\beta|v_2\rangle \\
\langle c_1v_1 + c_2v_2|\beta\rangle &= c_1^*\langle v_1|\beta\rangle + c_2^*\langle v_2|\beta\rangle
\end{aligned}$$

Definition. (Operator algebra) Notice that operators form a ring with an underlying structure of a vector space which is exactly the definition of an algebra.

Remark. (Identities)

(i) $(A^\dagger)^\dagger = A$

(ii) $(AB)^\dagger = B^\dagger A^\dagger$

(iii) $(\alpha A)^\dagger = \alpha^* A^\dagger$

Proof. For (i), let $B = A^\dagger$.

$$\langle\phi, B^\dagger\psi\rangle = \langle B\phi, \psi\rangle = \langle\psi, B\phi\rangle^* = \langle\psi, A^\dagger\phi\rangle^* = \langle A\psi, \phi\rangle^* = \langle\phi, A\psi\rangle$$

This will be on the test! For (ii),

$$\langle \phi, (AB)^\dagger \psi \rangle = \langle AB\phi, \psi \rangle = \langle B\phi, A^\dagger \psi \rangle = \langle \phi, B^\dagger A^\dagger \psi \rangle$$

For (iii),

$$\langle \phi, (\alpha A)^\dagger \psi \rangle = \langle \alpha A\phi, \psi \rangle = \alpha^* \langle A\phi, \psi \rangle = \alpha^* \langle \phi, A^\dagger \psi \rangle$$

□

Theorem. (Eigenvalue problem for Hermitian operators) Let $A|\psi_n\rangle = a_n|\psi_n\rangle$ and $A|\psi_m\rangle = a_m|\psi_m\rangle$. Applying the dual of $|\psi_m\rangle$ and $|\psi_n\rangle$ each,

$$\langle \psi_m|A|\psi_n\rangle = a_n\langle \psi_m|\psi_n\rangle \quad \langle \psi_n|A|\psi_m\rangle = a_m\langle \psi_n|\psi_m\rangle$$

Taking the complex conjugate of the right, we have

$$\langle \psi_m|A^\dagger|\psi_n\rangle = \langle A\psi_m|\psi_n\rangle = \langle \psi_n|A\psi_m\rangle^* = a_m^*\langle \psi_m|\psi_n\rangle$$

We conclude that

$$a_m^*\langle \psi_m|\psi_n\rangle = a_n\langle \psi_m|\psi_n\rangle \quad \text{and} \quad (a_m^* - a_n)\langle \psi_m|\psi_n\rangle = 0$$

when $m = n$, due to the positive definiteness of the inner product, we conclude that the eigenvalues are real. When $m \neq n$, we require that the inner product is zero, which proves orthogonality. In conclusion, we have proved the for self-adjoint operators, eigenvalues are real and they form an orthonormal set. Whether they form a complete basis is another difficult problem which we take for granted.

Proposition. (Probability interpretation) For an observable quantity A measured with respect to $|\psi\rangle$, once a observation is made, one of $\{a_n\}$ is observed and the probability that this happens is $|a_n|^2$.

4 Lecture 18 (May 12th)

Proposition. The dynamics, or evolution of a quantum state is given by

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$$

whereas, because $\hat{H} = \hat{H}^\dagger$,

$$-i\hbar\frac{\partial}{\partial t}\langle\psi(t)| = \langle\psi(t)|\hat{H}$$

Definition. For any linear map $\hat{A} : V \to V$ between vector spaces, we can create a matrix representation according to

$$\hat{A}(\mathbf{e}_i) = \sum_j \mathbf{e}_j A_{ji} \quad \text{and} \quad \langle \mathbf{e}_j, \hat{A}(\mathbf{e}_i)\rangle = \sum_k A_{ki}\langle \mathbf{e}_j, \mathbf{e}_k\rangle = \sum_k A_{ki}\delta_{jk} = A_{ji}$$

with respect to the basis $\{\mathbf{e}_i\}$. Now, let $\mathcal{H}$ be a Hilbert space with respect to $\{|n\rangle\}$. For an operator $\hat{A} : \mathcal{H} \to \mathcal{H}$, we have

$$\hat{A}|n\rangle = \sum_n A_{mn}|m\rangle \quad \text{or} \quad \langle m|\hat{A}|n\rangle = A_{mn}$$

Now, by extension, we can create a matrix representation for any operator by employing the completeness relation

$$\hat{A} = \mathbf{1}\hat{A}\mathbf{1} = \sum_{n,m} |n\rangle\langle n|\hat{A}|m\rangle\langle m| = \sum_{m,n} A_{nm}|n\rangle\langle m|$$

In the language of matrices, for any inner product, we can express

$$\langle\Phi|\Psi\rangle = \langle\Phi|\sum_n |n\rangle\langle n|\Psi\rangle = \sum_n \langle\Phi|n\rangle\langle n|\Psi\rangle = \sum_n (\langle 1|\Phi\rangle^*, \langle 2|\Phi\rangle^*, \ldots)\begin{pmatrix}\langle 1|\Psi\rangle \\ \langle 2|\Psi\rangle \\ \vdots\end{pmatrix}$$

Therefore, kets can be seen as column vectors while bras can be seen as complex conjugated and transposed rows. Likewise, the dual relationship between the Hermitian and row vectors are parallel to the dual relation between bras and kets.

Example. (Quantum gates) We now learn the NOT quantum gate $\hat{O} : \mathbf{C}^2 \to \mathbf{C}^2$. If suffices to define the linear function on the basis like the following:

$$\begin{cases}\hat{O}|0\rangle = |1\rangle \\ \hat{O}|1\rangle = |0\rangle\end{cases}$$

We can now find the matrix representation using the formalism above,

$$\begin{aligned} A_{11} &= \langle 0|\hat{O}|0\rangle = 0 \quad & A_{12} &= \langle 0|\hat{O}|1\rangle = 1 \\ A_{21} &= \langle 1|\hat{O}|0\rangle = 1 \quad & A_{22} &= \langle 1|\hat{O}|1\rangle = 0 \end{aligned}$$

Where we get

$$\hat{A} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \text{or} \quad \hat{A} = |1\rangle\langle 0| + |0\rangle\langle 1|$$

Definition. The Pauli matrices are defined like the following

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Note that they are Hermitian, unitary, and has a trace of 0.

Definition. (Mixed state) A general (or mixed) quantum state $\rho : \mathcal{H} \to \mathcal{H}$ is defined as an operator that is

(i) Hermitian

(ii) $\mathrm{Tr}(\rho) = 1$

(iii) Positive operator (also called a positive semidefinite operator), meaning $\langle\psi|\rho|\psi\rangle \geq 0$ for all $|\psi\rangle$

A general quantum state is also called a density operator.

Definition. In the Dirac sense, the wavefunctions $\psi(x)$ and $\phi(x)$ in the position space and the momentum space respectively are the coefficents of the state vector when projected into the position space and momentum space respectively. That is, by defining the eigenstates $|x\rangle$ and $|p\rangle$ to form a generalised orthonormal basis satisfying the following condition,

$$\langle x|x'\rangle = \delta(x - x')$$

states can be expanded as

$$|\psi\rangle = \int_{-\infty}^{\infty} dx'\, \psi(x')|x'\rangle \quad |\psi\rangle = \int_{-\infty}^{\infty} dp'\, \phi(p')|p'\rangle$$

with

$$\langle x|\psi\rangle = \int_{-\infty}^{\infty} dx'\, \psi(x')\langle x|x'\rangle = \int_{-\infty}^{\infty} dx'\, \psi(x')\delta(x - x') = \psi(x)$$

and likewise for the momentum function.

5 Lecture 19 (May 14th)

Lemma. We first try to obtain $\langle x|p\rangle$ and $\langle p|x\rangle$. Notice that

$$\langle x|\hat{p}|p\rangle = p\langle x|p\rangle = -i\hbar\frac{d}{dx}\langle x|p\rangle$$

Solving the differential equation we find

$$\langle x|p\rangle = A(p)e^{ipx/\hbar}$$

Noting the identity

$$\int_{-\infty}^{\infty} dx\, e^{ikx} = 2\pi\delta(k)$$

we find

$$\begin{aligned}
\langle p|p'\rangle =& \delta(p-p') \\
\int_{-\infty}^{\infty} dx\, \langle p|x\rangle\langle x|p'\rangle =& \delta(p-p') \\
\int_{-\infty}^{\infty} dx\, |A(p)|^2 e^{ix(p-p')/\hbar} =& \delta(p-p') \\
|A(p)|^2 2\pi\delta\Big(\frac{p-p'}{\hbar}\Big) =& \delta(p-p') \\
A(p) =& \frac{1}{\sqrt{2\pi\hbar}}
\end{aligned}$$

Theorem. (Fourier transform) We find that the inverse Fourier and Fourier transforms are given as

$$\begin{aligned}
\psi(x) = \langle x|\psi\rangle &= \int_{-\infty}^{\infty} dp\, \langle x|p\rangle\langle p|x\rangle \\
&= \int_{-\infty}^{\infty} dp\, e^{ipx/\hbar}\frac{1}{\sqrt{2\pi\hbar}}\phi(p)
\end{aligned}$$

and

$$\phi(p) = \langle p|\psi\rangle = \int_{-\infty}^{\infty} dx\, e^{ipx/\hbar}\frac{1}{\sqrt{2\pi\hbar}}\psi(x)$$

Remark.

Proposition. (Matrix representation) We can express the below basis independent expression of an arbitrary linear transformation in terms of matrices,

$$|\psi\rangle = A|\phi\rangle$$

by projecting into the basis $\langle m|$ and inserting the completeness relation,

$$\langle m|\psi\rangle = \sum_n \langle m|A|n\rangle\langle n|\phi\rangle \quad \text{or} \quad \psi_m = \sum_n A_{mn}\phi_n$$

where ϕ_m and ϕ_n are ordinary matrices. On the other hand,

$$A = BC$$

can be expressed as

$$\langle m|A|n\rangle = \sum_k \langle m|B|k\rangle\langle k|C|n\rangle \quad \text{or} \quad A_{mn} = \sum_k B_{mk}C_{kn}$$

Remark. (Adjoint matrices) We now seek the matrix expression for an adjoint operator.

$$(A_{nm})^\dagger = \langle n|A^\dagger|m\rangle = \langle An|m\rangle = \langle m|An\rangle^* = (\langle m|A|n\rangle)^* = A^*_{mn}$$

We find that an adjoint of an operator in terms of its matrix is simply the complex transpose of the operator itself.

Definition. (Unitary operators) A key property of unitary operators (operators satisfying $O^\dagger O = OO^\dagger = \mathbf{1}$) is that they preserve inner products. This can be seen from the fact that as $|\phi\rangle \to U|\phi\rangle$ and $|\psi\rangle \to U|\psi\rangle$,

$$\langle U\psi|U\phi\rangle = \langle \psi|U^\dagger U|\phi\rangle$$

Definition. (Trace) The trace of a matrix is defined like the following

$$\mathrm{Tr}(A) = \sum_n \langle n|A|n\rangle = \sum_n A_{nn}$$

However, see how the definition relies of a certain basis $\{|n\rangle\}$. We now prove that the definition is independent on this set. Take another basis $\{|m\rangle\}$. We see that

$$\begin{aligned}
\sum_n \langle n|A|n\rangle &= \sum_{n,m_1,m_2} \langle n|m_1\rangle\langle m_1|A|m_2\rangle\langle m_2|n\rangle \\
&= \sum_{n,m_1,m_2} \langle m_1|A|m_2\rangle\langle m_2|n\rangle\langle n|m_1\rangle \\
&= \sum_{m_1,m_2} \langle m_1|A|m_2\rangle\delta_{m_1m_2}
\end{aligned}$$

Definition. (Spectral decomposition of a Hermitian operator) Consider a Hermitian operator

$$\hat{A} = \sum_{n,m} |n\rangle\langle n|A|m\rangle\langle m|$$

and select the basis to be eigenkets of $\hat{A}$. We have

$$\langle n|\hat{A}|m\rangle = \langle n|A_m|m\rangle = A_m\langle n|m\rangle = A_m\delta_{nm}$$

When inserting this into the above, we diagonalise the matrix by obtaining

$$\sum_m |m\rangle A_m\langle m|$$

We see that the eigenvalues form the diagonals of the Hermitian matrix.

Theorem. (Operator solution of the simple harmonic oscillator) We have previously witnessed the simple harmonic oscillator whose Hamiltonian was given by

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$$

We are certain that $\langle\psi|\hat{H}|\psi\rangle \geq 0$ from the fact that $\langle\psi|\hat{x}\hat{x}|\psi\rangle = \langle\hat{x}^\dagger\psi|\hat{x}\psi\rangle \geq 0$. Define the following operator

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + i\frac{\hat{p}}{\sqrt{2m\omega\hbar}}$$
$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} - i\frac{\hat{p}}{\sqrt{2m\omega\hbar}}$$

If possible, memorise these. Knowing that $[\hat{x},\hat{p}] = i\hbar$, we can compute that $[\hat{a},\hat{a}^\dagger] = \mathbf{1}$. We then find

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}+\hat{a}^\dagger) \quad \hat{p} = \dots$$

In terms of $\hat{a}$, we therefore find the Hamiltonian above to be (it is extremely important to be careful of the order of $\hat{a}$ and $\hat{a}^\dagger$):

$$\hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)$$

What is the commutator relation between $\hat{H}$ and $\hat{a}$? We see that

$$[H,a] = \hbar\omega\left[a^\dagger a + \frac{1}{2}a\right] = \hbar\omega(a^\dagger[a,a] + [a^\dagger,a]a) = \hbar\omega(-a) \quad \text{with} \quad [H,a^\dagger] = \hbar\omega a^\dagger$$

Physically, each operator is defined as operators that raise and lowers energy levels. Now we actually solve for energy levels.

$$\hat{H}|E\rangle = E|E\rangle$$
$$\hat{H}(a|E\rangle) = (aH + [\hat{H},a])|E\rangle = (\hat{a}E - \hbar\omega\hat{a})|E\rangle = (E-\hbar\omega)(\hat{a}|E\rangle)$$

6 Lecture 20 (May 19th)

Theorem. Let there be an energy state $\hat{H}|E\rangle = E|E\rangle$. We previously found how

$$\hat{H}(\hat{a}|E\rangle) = (E-\hbar\omega)(\hat{a}|E\rangle)$$

and

$$\hat{H}(a^\dagger|E\rangle) = (E+\hbar\omega)(\hat{a}^\dagger|E\rangle)$$

Which needs to be verified. We have previously proved

$$\langle\psi|\hat{H}|\psi\rangle \geq 0$$

and tells us that there is a limit to how much the energy can be lowered. We thus define

$$\hat{a}|0\rangle = \mathbf{0}$$

as the ground state, where $\mathbf{0}$ is the zero vector. A simple corollary would be that

$$\hat{H}|0\rangle = (\hbar\omega)(\hat{a}^\dagger\hat{a})|0\rangle = \frac{1}{2}\hbar\omega|0\rangle$$

telling us that the ground state has an energy of $\hbar\omega/2$. We can apply the creation operator to obtain higher energy states:

$$H(\hat{a}^\dagger|0\rangle) = \left(\frac{1}{2}\hbar\omega + \hbar\omega\right)(\hat{a}^\dagger|0\rangle)$$

For arbitrary states,

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

and

$$|n\rangle = c_n(\hat{a}^\dagger)^n|0\rangle$$

We now prove that these eigenvectors form an orthonormal basis. The inner product of two eigenstates are

$$\langle m|n\rangle = c_m^* c_n\langle 0|a^m(a^\dagger)^n|0\rangle = c_m^* c_n n\langle 0|a^{m-1}(a^\dagger)^{n-1}|0\rangle$$

as $a^{m-1}a(a^\dagger)^n = ((a^\dagger)^n)a + [a,(a^\dagger)^n]) = ((a^\dagger)^n a + n(a^\dagger)^{n-1})$. Therefore, when $n \neq m$, we find $\langle n|m\rangle = 0$ and if they are equal,

$$\langle n|m\rangle = |c_n|^2 n\langle 0|a^{n-1}(a^\dagger)^{n-1}|0\rangle = |c_n|^2 n(n-1)\langle 0|a^{n-1}(a^\dagger)^{n-2}|0\rangle = \ldots = |c_n|^2 n!\langle 0|0\rangle = 1$$

thus getting something we should definitely memorise,

$$|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n|0\rangle$$

with $\langle n|m\rangle = \delta_{nm}$. Let's not find the annihilator operators matrix representation.

$$\begin{aligned}\langle m|a|n\rangle =&\langle m|a\cdot\frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle = \frac{1}{\sqrt{n!}}\langle m|(a^\dagger)^n a + a(a^\dagger)^n|0\rangle\\ =&\frac{n}{\sqrt{n!}}\langle m|(a^\dagger)^{n-1}|0\rangle = \frac{n}{\sqrt{n!}}\sqrt{(n-1)!}\langle m|\frac{(a^\dagger)^{n-1}}{\sqrt{(n-1)!}}|0\rangle\\ =&\sqrt{n}\,\delta_{m,n-1}\end{aligned}$$

We can use the above to also obtain the creator operator's matrix representation, where

$$\langle m|\hat{a}^\dagger|n\rangle = \langle\hat{a}m|n\rangle = \langle n|a|m\rangle^* = (\delta_{n,m-1}\sqrt{m})^* = \delta_{n,m-1}\sqrt{m} = \delta_{m+1,n}\sqrt{n+1}$$

Theorem. What is the wavefunction of the ground state? Mathematically, what is $\psi_0 = \langle x|0\rangle$?

$$\hat{a}|0\rangle = 0 \to \Big(\sqrt{\frac{m\omega}{2\hbar}}\hat{x} + i\sqrt{\frac{1}{2m\omega\hbar}}\hat{p}\Big)|0\rangle = 0$$

which leads to

$$\Big[\sqrt{\frac{m\omega}{2\hbar}}x + i\sqrt{\frac{1}{2m\omega\hbar}}\Big(-i\hbar\frac{d}{dx}\Big)\Big]\langle x|0\rangle = 0$$

and

$$\langle x|0\rangle = c\exp\Big(-\frac{m\omega x^2}{2\hbar}\Big)$$

which must be normalised with

$$\int_{-\infty}^{\infty} |\langle x|0\rangle|^2 = 1 \quad \text{and} \quad c = \Big(\frac{m\omega}{\pi\hbar}\Big)^{1/4}$$

To find higher wave functions,

$$\psi_n(x) = \langle x|n\rangle$$

try and compute this with $n = 1$.

Definition. Define the exponential of an operator as

$$\exp(\hat{A}) = \sum_{n=0}^{\infty}\frac{1}{n!}(\hat{A})^n$$

Define the operator $\hat{U} = \exp(i\hat{A})$ for a Hermitian $\hat{A}$. We find that

$$\hat{U}^\dagger = (\sum_{n=0}^{\infty}(-i)^n\hat{A}^n) = \exp(-i\hat{A}) = \hat{U}^{-1}$$

Therefore,

$$\hat{U}^\dagger\hat{U} = \mathbf{1}$$

and $\hat{U}$ is a unitary operator.

Theorem. (Commuting set of operators and degeneracy) Here, we consider Hilbert spaces that are completely spanned by eigenstates of Hermitian operators. Take

$$\hat{A}|u_a\rangle = a|u_a\rangle$$

which also satisfies

$$\hat{B}|u_a\rangle = b|u_a\rangle$$

Completeness dictates that

$$\sum_{a,b}|u_{ab}\rangle\langle u_{ab}| = \mathbf{1}$$

then,

$$[\hat{A}, \hat{B}]|u_{ab}\rangle = (\hat{A}\hat{B} - \hat{B}\hat{A})|u_{ab}\rangle = (ab - ba)|u_{ab}\rangle = 0$$

telling us that $[\hat{A}, \hat{B}] = 0$.

7 Lecture 21 (May 21st)

Theorem. (Exsistence of simultaneous eigenkets for commuting operators) Let $[\hat{A}, \hat{B}] = 0$, that is, $\hat{A}$ and $\hat{B}$ be commuting operators. Consider the set of eigenstates $\{|u_a\rangle\}$ of $\hat{A}$, satisfying

$$\hat{A}|u_a\rangle = a|u_a\rangle$$

Observe that

$$\hat{A}(\hat{B}|u_a\rangle) = \hat{B}(\hat{A}|u_a\rangle) = a(\hat{B}|u_a)$$

How many eigenkets (eigenstates) does the eigenvalue a have? Assume that it has 1 and we have:

$$\hat{B}|u_a\rangle = b|u_a\rangle$$

where $|u_a\rangle$ is a simultaneous eigenket for both $\hat{A}$ and $\hat{B}$. In this case, we say that the eigenvalue is nondegenerate. Assume that it has 2, $|u_a^{(1)}\rangle$ and $|u_a^{(2)}\rangle$. Applying the operator $\hat{B}$, we expect

$$\begin{cases} \hat{B}|u_a^{(1)}\rangle = c_{11}|u_a^{(1)}\rangle + c_{21}|u_a^{(2)}\rangle \\ \hat{B}|u_a^{(2)}\rangle = c_{21}|u_a^{(1)}\rangle + c_{22}|u_a^{(2)}\rangle \end{cases}$$

As $\hat{B}$ is Hermitian, the following matrix would have a diagonal form,

$$\begin{pmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{pmatrix} \longrightarrow \begin{pmatrix} \lambda_b^{(1)} & 0 \\ 0 & \lambda_b^{(2)} \end{pmatrix}$$

By which we conclude

$$\begin{cases} \hat{B}|v_a^{(1)}\rangle = \lambda_b^{(1)}|v_a^{(1)}\rangle \\ \hat{B}|v_a^{(2)}\rangle = \lambda_b^{(2)}|v_a^{(1)}\rangle \end{cases}$$

for some vectors $|v_a^{(i)}\rangle$. We therefore find $|u_a\rangle$ to be simultaneous eigenkets of $\hat{A}$ and $\hat{B}$. In this case, we say that the eigenvalue is degenerate.

Definition. (Expectation values) Consider the expectation value of $\hat{A}$, defined as

$$\langle\psi(t)|\hat{A}|\psi(t)\rangle$$

For kets, the Schrodinger equation is given as

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$$
$$-i\hbar\frac{\partial}{\partial t}\langle\psi(t) = \langle\psi(t)|\hat{H}$$

For now, we take $\hat{H}$ to be time-independent. We find

$$\begin{aligned}\frac{d}{dt}\Big(\langle\psi(t)|\hat{A}|\psi(t)\rangle\Big) =&\Big(\frac{d}{dt}\langle\psi(t)|\Big)\hat{A}|\psi(t)\rangle + \langle\psi(t)|A\Big(\frac{d}{dt}|\psi(t)\rangle\Big) + \langle\psi(t)|\frac{\partial A}{\partial t}|\psi(t)\rangle \\ =&\frac{i}{\hbar}\langle\psi(t)|[\hat{H},\hat{A}]|\psi(t)\rangle + \langle\psi(t)|\frac{\partial A}{\partial t}|\psi(t)\rangle\end{aligned}$$

From this we learn that expectation values (given that the observable is time independent) are only conserved through time when the commutator with the Hamiltonian operator is 0.

$$[\hat{A},\hat{H}] = 0$$

Example. (Ehrenfest theorem) Take $\hat{A} = \hat{x}$ and

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$$

The derivative of the expectation value is given as

$$\frac{d}{dt}\langle\hat{x}\rangle = \frac{i}{\hbar}\langle\psi|[H,\hat{x}]|\psi\rangle = \Big\langle\frac{\hat{p}}{m}\Big\rangle$$

On the other hand,

$$\frac{d}{dt}\langle\hat{p}\rangle = \frac{i}{\hbar}\langle\psi|[\hat{H},\hat{p}]|\psi\rangle = -\Big\langle\frac{dV}{dx}\Big\rangle$$

Derivating the top equation one more time,

$$m\frac{d^2}{dt^2}\langle\hat{x}\rangle = \frac{d}{dt}\langle\hat{p}\rangle = -\Big\langle\frac{dV}{dx}\Big\rangle$$

we find the quantum mechanical version of Newton's theorem.

Definition. (Schrodinger and Heisenberg picture of quantum theory) Like the above, when we take wavefunctions to be time independent, we call the construction Schrodinger's picture of quantum mechanics. On the other hand, suppose that time evolution is introduced by

$$|\psi(t)\rangle = \exp\Big(-\frac{\hat{H}t}{\hbar}\Big)|\psi(0)\rangle$$

where we call the exponential term (an unitary operator) the time evolution operator. The time dependent ket satisfies the Schrodginer equation, as

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = i\hbar\Big(-\frac{i\hat{H}}{\hbar}\Big)\exp\Big(-\frac{i\hat{H}t}{\hbar}\Big)|\psi(0)\rangle = \hat{H}|\psi(t)\rangle$$

The expectation value, with this formulation, becomes

$$\langle\psi(0)|\exp\Big(\frac{i\hat{H}t}{\hbar}\Big)\hat{A}\exp\Big(-\frac{i\hat{H}t}{\hbar}\Big)|\psi(0)\rangle$$

In this case, we see how instead of the states, the operators evolve throughout time ($\hat{A} = \hat{A}(t)$), and quantum mechanics seen in this manner is called Heisenberg's picture. We emphasize that the above is a formal solution, meaning that we aren't caring about details. In this process, we care about the time derivative of $\hat{A_H}(t)$ which we find to be

$$\begin{aligned}
\frac{d}{dt}\hat{A_H}(t) =& \frac{i\hat{H}}{\hbar}\exp\Big(\frac{iHt}{\hbar}\Big)\hat{A}_S\exp\Big(-\frac{i\hat{H}t}{\hbar}\Big) + \exp\Big(\frac{iHt}{\hbar}\Big)\hat{A}_S\exp\Big(-\frac{iHt}{\hbar}\Big)\Big(-\frac{i\hat{H}}{\hbar}\Big) \\
&+ \exp\Big(\frac{i\hat{H}t}{\hbar}\Big)\frac{\partial A_S}{\partial t}\exp\Big(-\frac{i\hat{H}t}{\hbar}\Big) \\
=& \frac{i\hat{H}}{\hbar}\hat{A}_H(t) - \frac{i}{\hbar}A_H(t)\cdot\hat{H} \\
=& \frac{i}{\hbar}[\hat{H}, \hat{A}_H(t)] + \exp\Big(\frac{i\hat{H}t}{\hbar}\Big)\frac{\partial A_S}{\partial t}\exp\Big(-\frac{i\hat{H}t}{\hbar}\Big)
\end{aligned}$$

We the parallel between Schrodinger and Hamilton's equations, and Heisenberg's and Poisson's equation.

Proposition. Does the commutator relation $[\hat{x}(t), \hat{p}(t)] = i\hbar$ hold in Heisenberg's picture? We see that

$$\begin{aligned}
\hat{x}(t)\hat{p}(t) - \hat{p}(t)\hat{x}(t) =& \exp\Big(\frac{i\hat{H}t}{\hbar}\Big)\hat{x}\Big(-\frac{i\hat{H}t}{\hbar}\Big)\exp\Big(\frac{i\hat{H}t}{\hbar}\Big)\hat{p}\Big(-\frac{i\hat{H}t}{\hbar}\Big) \\
&- \exp\Big(\frac{i\hat{H}t}{\hbar}\Big)\hat{x}\Big(-\frac{i\hat{H}t}{\hbar}\Big)\exp\Big(\frac{i\hat{H}t}{\hbar}\Big)\hat{x}\Big(-\frac{i\hat{H}t}{\hbar}\Big) \\
=& \exp\Big(\frac{i\hat{H}t}{\hbar}\Big)(\hat{x}\hat{p} - \hat{p}\hat{x})\Big(-\frac{i\hat{H}t}{\hbar}\Big) \\
=& i\hbar
\end{aligned}$$

It is then important to check that $[\hat{a}, \hat{a}^\dagger] = 1$ too!

8 Lecture 22 (May 26th)

Remark. Last class we have learned the time derivative of an operator in Heisenberg's picture, given by

$$\frac{d}{dt}\hat{A}_H(t) = \frac{i}{\hbar}[\hat{H}, \hat{A}_H(t)] + \exp\Big(\frac{i\hat{H}t}{\hbar}\Big)\frac{\partial\hat{A}_S}{\partial t}(t_{\rm s})\exp\Big(-\frac{i\hat{H}t}{\hbar}\Big)$$

The hamilotian in the Heisenberg picture is

$$\hat{H}_H = \exp\Big(\frac{i\hat{H}_S t}{\hbar}\Big)\hat{H}_S\exp\Big(-\frac{i\hat{H}_S t}{\hbar}\Big) = \hat{H}_S$$

from the fact that $[H^n, H] = H^nH - HH^n = 0$.

Theorem. (Harmonic oscillator) From $\hat{H}_S = \hbar\omega(\hat{a}^\dagger\hat{a} + 1/2) = \hbar\omega(\hat{a}^\dagger(t)\hat{a}(t) + 1/2) = \hat{H}_H$

we find

$$\begin{aligned}
\frac{d\hat{a}(t)}{dt} =& \frac{i}{\hbar}[\hat{H}, \hat{a}(t)] = i\omega[\hat{a}^\dagger(t)\hat{a}(t), \hat{a}(t)] \\
=& i\omega[\hat{a}^\dagger(t), \hat{a}(t)]\hat{a}(t) = -i\omega(t)\hat{a}(t)
\end{aligned}$$

Solving the following the differential equation we find

$$\hat{a}(t) = e^{-i\omega t}\hat{a}(0)$$

Preforming the adjoint,

$$\hat{a}^\dagger(t) = e^{i\omega t}\hat{a}^\dagger(0)$$

We can then seek (do this!) $\hat{x}(t)$ and $\hat{p}(t)$ and you will find dependence on $\hat{x}(0)$ and $\hat{p}(0)$ as if you solved the Newton's equations.

Example. Seek, for example,

$$\langle 0|\hat{a}(t)\hat{a}^\dagger(0)|0\rangle = e^{-i\omega t}\langle 0|\hat{a}(0)\hat{a}^\dagger(0)|0\rangle = e^{-i\omega t}$$

these functions are called correlation functions. Harmonic oscillators and angular momentum questions will be dealt in the final exam.

Proposition. Suppose you want to translate a wave function. Such a such that preforms this operation can be expressed as

$$\langle x|T(a)|\psi\rangle$$

where we want to move the wave function a to the right.

$$\begin{aligned}
\psi(x-a) =& \sum_{n=0}^{\infty} \frac{1}{n!}(-a)^n \frac{d^n}{dx^n}\psi(x) = \sum_{n=0}^{\infty} \frac{1}{n!}\Big(-\frac{ia}{\hbar}\Big)^n (-i\hbar)^n \frac{d^n}{dx^n}\psi(x) \\
=& \langle x| \sum_{n=0}^{\infty} \frac{1}{n!}\Big(-\frac{ia\hat{p}}{\hbar}\Big)^n |\psi\rangle = \langle x| \exp\Big(-\frac{ia\hat{p}}{\hbar}\Big)|\psi\rangle
\end{aligned}$$

we thus find the translation operator to be a unitary operator

$$T(a) = \exp\Big(-\frac{ia\hat{p}}{\hbar}\Big)$$

Definition. (Angular momentum) Angular momentum is classically given as

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}$$

We find that

$$\begin{cases} L_x = yP_z - zP_y \\ L_y = zP_x - xP_z \\ L_z = xP_y - yP_x \end{cases}$$

Finding the comutators,

$$\begin{aligned}
[L_x, L_y] =& [yP_z - zP_y, zP_x - xP_z] \\
=& (yP_z - zP_y)(zP_x - xP_z) - (zP_x - xP_z)(yP_z - zP_y) \\
=& [yP_z, zP_x] - [yP_z, xP_z] - [zP_y, zP_x] + [zP_y, xP_z] \\
=& y[P_z, z]P_x - y[P_z, P_z]x - P_y[z, z]P_x + x[zP_y, P_z] + [zP_y, x]P_z \\
=& y(-i\hbar)P_x + x(i\hbar)P_y = i\hbar L_z
\end{aligned}$$

as

$$x[zP_y, P_z] + [zP_y, x]P_z = x(z[P_y, P_z] + (i\hbar)P_y)$$

Along this line,

$$[L_x, L_y] = i\hbar L_z \quad [L_y, L_z] = i\hbar L_x \quad [L_z, L_x] = i\hbar L_y$$

and we have

$$[L_a, L_b] = i\hbar\epsilon_{abc}L_c$$

with $(a, b, c) = (x, y, z)$. This forms a $SU(2)$ Lie algebra, and applies to spin also. Now take

$$\mathbf{L} \cdot \mathbf{L} = L_x^2 + L_y^2 + L_z^2$$

Finding the commutator with L_z,

$$[\mathbf{L} \cdot \mathbf{L}, L_z] = [L_x^2 + L_y^2, L_z] = [L_x^2, L_z] + [L_y^2, L_z] = 0$$

where

$$[L_x^2, L_z] = L_x[L_x, L_z] + [L_x, L_z]L_x = L_x(-i\hbar L_y) + (-i\hbar L_y)L_x$$

and

$$[L_y^2, L_z] = L_y[L_y, L_z] + [L_y, L_z]L_y = i\hbar L_y L_x + i\hbar L_x L_y$$

In quantum physics, we choose $\mathbf{L}^2$ and L_z to be the commuting set with simulataneous eigenkets $|l, m\rangle$, which we define to satisfy the equations

$$\mathbf{L}^2|l, m\rangle = \hbar^2 l(l+1)|l, m\rangle \quad \text{and} \quad L_z|l, m\rangle = \hbar m|l, m\rangle$$

From here, we see that

$$\langle l, m|\mathbf{L} \cdot \mathbf{L}|l, m\rangle = \hbar l(l+1) = \langle L_x lm|L_x lm\rangle + \ldots \geq 0$$

and we impose that $l \geq 0$. As $|l, m\rangle$ are eigenkets, we have

$$\langle l', m' | l, m\rangle = \delta_{ll'}\delta_{mm'}$$

These calculations are 1000% in the exams and must be memorised.

Remark. We now investigate

$$\begin{cases} L_+ = L_x + iL_y \\ L_- = L_x - iL_y \end{cases}$$

$[\mathbf{L}^2, L_\pm] = 0$ is trivial, meanwhile

$$[L_z, L_+] = \hbar L_+ \quad [L_z, L_-] = -\hbar L_-$$

9 Lecture 23 (May 28th)

Recall. Last time we have learned that

$$[L_i, L_j] = i\hbar\varepsilon_{ijk}L_k$$

and that for $\mathbf{L}^2 = L_x^2 + L_y^2 + L_z^2$ and $L_\pm = L_x \pm iL_y$, the following identities hold.

$$\begin{cases} [\mathbf{L}^2, L_a] = 0 & [L_z, L_+] = \hbar L_+ \\ [L_+, L_-] = 2\hbar L_z & [L_z, L_-] = -\hbar L_- \end{cases}$$

Also, we defined the simultaneous eigenvectors $|l, m\rangle$ to satifisfy

$$\mathbf{L}^2|l, m\rangle = \hbar^2 l(l+1)|l, m\rangle \quad \text{and} \quad L_z|l, m\rangle = m\hbar|l, m\rangle$$

We notice that from $[\mathbf{L}^2, L_a] = 0$, we have $[\mathbf{L}^2, L_\pm] = 0$, or

$$\mathbf{L}^2(L_+|l, m\rangle) = L_+\mathbf{L}^2|l, m\rangle = l(l+1)\hbar^2(L_+|l, m\rangle)$$

Therefore, $L_+|l, m\rangle$ belongs to the l-multiplet. Continuing,

$$\begin{aligned} L_z(L_+|l, m\rangle) =& ([L_z, L_+] + L_+L_z)|l, m\rangle \\ =& (\hbar L_+ + m\hbar L_+)|l, m\rangle \\ =& (m+1)\hbar(L_+|l, m\rangle) \end{aligned}$$

From this we obtain the fact that

$$L_+|l, m\rangle = C_{lm}^+|l, m+1\rangle \quad \text{or} \quad L_-|l, m\rangle = C_{lm}^-|l, m-1\rangle$$

Taking the dual of the first,

$$\langle l, m| L_- = (C^+_{lm})^* \langle l, m+1|$$

Applying this to the ket $|l, m\rangle$,

$$\langle l, m| L_- L_+ |l, m\rangle = |C^+_{lm}|^2 \langle l, m+1 | l, m+1\rangle$$

The operator on the left is equal to $\mathbf{L}^2 - L_z^2 - \hbar L_z$. We then have

$$|C^+_{lm}|^2 = \hbar^2 (l-m)(l+m+1)$$

and further that

$$C^+_{lm} = \pm \hbar \sqrt{(l-m)(l+m+1)}$$

where we take the positive sign. On the other hand,

$$C^-_{lm} = \hbar \sqrt{(l+m)(l-m+1)}$$

you MUST do this. Now we have accumulated the following facts

$$\begin{cases} l \geq 0 \\ l(l+1) - m(m+1) \geq 0 \\ l(l+1) - m(m-1) \geq 0 \end{cases}$$

From this we obtain that

$$-l \leq m \leq l$$

which must be memorised. We lastly remark that operators like $\mathbf{L}^2$ are Casimir operators.

Corollary. We now have that

(i) $l \geq 0$

(ii) $-l \leq m \leq l$

(iii) m has a minimum value m_{min}, abeit that it doesn't have to be $-l$

$$L_- |l, m_{\text{min}}\rangle = 0 = C^-_{l, m_{\text{min}}} |l, m_{\text{min}} - 1\rangle$$

which tells us that $C^-_{l, m_{\text{min}}} = 0$. In otherwords,

$$\sqrt{(l + m_{\text{min}})(l - m_{\text{min}} + 1)} = 0$$

which teaches us that m_{min} is exactly $-l$. You should separately prove that identically, m has a maximum of $m_{\text{max}} = +l$. Do this calculation.

(iv) m has a maximum value $m_{\text{max}} = l$

(v) The possible values of l values are given as $l \in \boldsymbol{Z} \cup \frac{1}{2}\boldsymbol{Z} \cup \{0\}$. We often write l for integers, s for fractional values, or j altogether.

Theorem. Now we seek the matrix representation of these operators. Consider the following for $\langle l', m'|\hat{O}|l, m\rangle$:

(i) $\hat{O} = \mathbf{L}^2$, $l(l+1)\hbar\langle l', m'|l, m\rangle = l(l+1)\hbar^2\delta_{ll'}\delta_{mm'}$

(ii) $\hat{O} = L_z$, $m\hbar\delta_{ll'}\delta_{mm'}$

(iii) $\hat{O} = L_+$, $C^+_{lm}\delta_{ll'}\delta_{m'm+1}$ and therefore is not diagonal

Definition. (Conserved quantities) Consider, for $\partial\hat{O}_S/\partial t$, the Heisenberg equation

$$\frac{d\hat{O}_H}{dt} = \frac{i}{\hbar}[H, \hat{O}_H]$$

For $\hat{O}_H$ to be a conserved quantity,

$$\frac{d\hat{O}_S}{dt} = 0 \quad \Longleftrightarrow \quad [H, \hat{O}_H] = 0$$

Theorem. We found that the momentum operator was the generator of the unitary translational operator,

$$T(\mathbf{a}) = \exp\Big(-\frac{i\mathbf{p}\cdot\mathbf{a}}{\hbar}\Big)$$

with $T(\mathbf{a})|\mathbf{x}\rangle = |\mathbf{x}+\mathbf{a}\rangle$. Along this logic, what is the momentum operator $\mathbf{L}$ the generator of? We expect it to be rotation!

Proof. For a small rotation counter clock-wise,

$$\begin{cases} x' = x\cos\theta - y\sin\theta \approx x - y\theta \\ y' = x\sin\theta + y\cos\theta \approx x\theta + y \end{cases}$$

Then, the wave function can be expressed as

$$\begin{aligned}
\psi(x', y') =& \psi(x - y\theta, y + x\theta) \\
=& \psi(x, y) - y\theta\frac{\partial\psi}{\partial x} + x\theta\frac{\partial\psi}{\partial y} \\
=& \psi(x, y) - y\theta\Big(\frac{i}{\hbar}\Big)(-i\hbar)\frac{\partial\psi}{\partial x} + x\theta\Big(\frac{i}{\hbar}\Big)(-i\hbar)\frac{\partial\psi}{\partial y} \\
=& \frac{i\theta}{\hbar}\langle x, y|(-yP_x + xP_y)|\psi\rangle
\end{aligned}$$

We thus have found that the angular momentum operator is the generator of the unitary rotation operator.

$$U(\hat{n},\theta) = \exp\Big(-\frac{i\mathbf{J}\cdot\mathbf{n}\theta}{\hbar}\Big)$$

$\square$

10 Lecture 24 (June 2nd)

Recall. We have the following operators generating the time, translation, and rotation groups.

$$U_{\text{time}} = \exp\Big(-i\frac{Ht}{\hbar}\Big) \qquad U_{\text{tran}} = \exp\Big(-i\frac{\mathbf{p}\cdot\mathbf{a}}{\hbar}\Big) \qquad U_{\text{rot}} = \exp\Big(-i\frac{\mathbf{J}\cdot\mathbf{n}\,\theta}{\hbar}\Big)$$

Proposition. For the orbital angular momentum, we consider the transformation from cartesian to cylindrical coordinates

$$\mathbf{L} = \mathbf{r}\times\mathbf{p}$$

with $(x,y,z)\to(r,\theta,\phi)$ through

$$\begin{cases} x = r\sin\theta\cos\phi \\ y = r\sin\theta\sin\phi \\ z = r\cos\theta \end{cases}$$

In the infinitesimal sense,

$$L_z = xP_y - yP_x = x\Big(i\hbar\frac{\partial}{\partial y}\Big) - y\Big(-i\hbar\frac{\partial}{\partial x}\Big) = -i\hbar\frac{\partial}{\partial\phi}$$

which should be calculated atleast once. By extension, we can also express $L_\pm$ in cartesian coordinates. Lastly, we can find $\mathbf{L}^2 = L_x^2 + L_y^2 + L_z^2$ to be

$$\mathbf{L}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\Big(\sin\theta\frac{\partial}{\partial\theta}\Big) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$

which is the Laplacian in terms of spherical coordinates.

Theorem. Memorize, again,

$$L_z|l,m\rangle = m\hbar|l,m\rangle \quad \text{and} \quad \mathbf{L}^2|l,m\rangle = l(l+1)\hbar^2|l,m\rangle$$

We define spherical harmonics as

$$\langle\theta,\phi|l,m\rangle = Y_{l,m}(\theta,\phi)$$

We can write

$$\int d\mathbf{x}\,|\mathbf{x}\rangle\langle\mathbf{x}| = \mathbf{1} \quad \text{and} \quad \int d\Omega\,|\theta,\phi\rangle\langle\theta,\phi| = \mathbf{1}$$

Then,

$$\int \sin\theta d\theta d\phi\,|\theta,\phi\rangle\langle\theta,\phi|\theta',\phi'\rangle$$

We then require that

$$\langle\theta,\phi|\theta',\phi'\rangle = \frac{\delta(\theta-\theta')\delta(\phi-\phi')}{\sin\theta} = \delta(\cos\theta-\cos\theta')\delta(\phi-\phi')$$

We now seek

$$\langle\theta,\phi|\hat{L}_z|l,m\rangle = m\hbar\langle\theta,\phi|l,m\rangle$$

implying

$$-i\hbar\frac{\partial}{\partial\phi}\langle\theta,\phi|l,m\rangle = m\hbar\langle\theta,\phi|l,m\rangle$$

and

$$\frac{\partial}{\partial\phi}Y_{l,m}(\theta,\phi) = imY_{l,m}(\theta,\phi)$$

We now know that $Y_{l,m}(\theta,\phi) = e^{im\phi}F(\theta)/\sqrt{2\pi}$ with m an integer, as the function should be periodic with respect to ϕ. We now use the operator $\mathbf{L}^2$ to determine $F(\theta)$.

$$\langle\theta,\phi|\mathbf{L}^2|l,m\rangle = l(l+1)\hbar^2\langle\theta,\phi|l,m\rangle$$

We have

$$-\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\Big(\sin\theta\frac{\partial}{\partial\theta}\Big) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\frac{e^{im\phi}}{\sqrt{2\pi}}F_{l,m}(\theta) = l(l+1)\hbar^2\frac{e^{im\phi}}{\sqrt{2\pi}}F_{l,m}(\theta)$$

and

$$-\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\Big(\sin\theta\frac{\partial}{\partial\theta}\Big) - \frac{m^2}{\sin^2\theta}\right]F_{l,m}(\theta) = l(l+1)F_{l,m}(\theta)$$

This is the associated Legendre polynomial with $m \neq 0$ (Legendre if $m = 0$). Finite solutions with $0 \leq \theta \leq \pi$ require that $l \geq 0$ and $l \in \boldsymbol{Z}$.

$$F_{l,m}(\theta) = P_{l,m}(\cos\theta)$$

Substituting $z = \cos\theta$, we have the more famililar

$$\frac{d}{dz}\Big[(1-z^2)\frac{dP_{l,m}}{dz}\Big] + \Big[l(l+1) - \frac{m^2}{1-z^2}\Big]P_{l,m} = 0$$

with solutions

$$P_{l,m}(z) = (1-z^2)^{m/2}\frac{d^m}{dz^m}P_l$$

Normalisation can be done through setting

$$\langle l', m'|l, m\rangle = \delta_{ll'}\delta_{mm'}$$

We have, then,

$$\int d\Omega \langle l', m'|\theta, \phi\rangle\langle\theta, \phi|l, m\rangle = \int d\Omega\, Y^*_{l',m'}(\theta, \phi)Y_{l,m}(\theta, \phi) = \delta_{ll'}\delta_{mm'}$$

and set coefficients accordingly. Resultantly,

$$Y_{l,m}(\theta, \phi) = (-1)^m \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}} P_{l,m}(\cos\theta)e^{im\phi}$$

for $m \geq 0$ and

$$Y_{l,-m} = (-1)^m (Y_{l,m})^*$$

for $m < 0$.

Corollary. Consider

$$\sum_{l,m} \langle\theta', \phi'|l, m\rangle\langle l, m|\theta, \phi\rangle = \sum_{l,m} Y_{l,m}(\theta', \phi')Y^*_{l,m}(\theta, \phi) = \langle\theta', \phi'|\theta, \phi\rangle = \frac{\delta(\theta - \theta')\delta(\phi - \phi')}{\sin\theta}$$

this is called the closure relation.

Definition. The parity operator was defined as the operator that sends $\mathbf{x} \to -\mathbf{x}$. How does this work in spherical polar coordinates? We require that

$$\theta \to \pi - \theta \quad \text{and} \quad \phi \to \phi + \pi$$

This turns $\cos\theta \to -\cos\theta$, and to an extension,

$$Y_{l,m}(-\mathbf{n}) = (-1)^l Y_{l,m}(\mathbf{n})$$

under parity.

11 Lecture 25 (June 4th)

Theorem. In spherical polar coordinates, the Hamiltonian is given as

$$\hat{H} = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}) = -\frac{\hbar^2}{2m}\nabla^2_{\mathbf{r}} + V(\mathbf{r})$$

The Laplacian in spherical coordinates is given as

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\underbrace{\Big(\frac{\partial^2}{\partial \theta^2} + \cot\theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial \phi^2}\Big)}_{-\mathbf{L}^2/\hbar^2}$$

We want to solve

$$\hat{H}\psi(r,\theta,\phi) = E\psi(r,\theta,\phi)$$

When solving a problem in QM, we need to first find all operators that commute with the Hamiltonian. For a potential that only depends on the modulus of the distance $V(|\mathbf{r}|)$, we can compute the commutator

$$[\mathbf{p}^2, L_z] = [p_x^2 + p_y^2 + p_z^2, xp_y - yp_x] = 0$$

check this later on. On the otherhand, we can compute the following,

$$\begin{aligned}[L_z, V(|\mathbf{r}|)] =& [xP_y - yP_x, V(|\mathbf{r}|) = x[P_y, V(|\mathbf{r}|)] - y[P_x, V(|\mathbf{r}|)] \\ =& x(-i\hbar)V'(|\mathbf{r}|)\frac{y}{r} - y(-i\hbar)V'(|\mathbf{r}|)\frac{x}{r} = 0\end{aligned}$$

In sum,

$$[H, L_z] = 0 \quad \text{and} \quad [H, \mathbf{L}^2] = 0$$

and there exists simultaneous eigenfunctions of H and L_z and $\mathbf{L}^2$. We previously saw that $Y_{l,m}(\theta,\phi)$ is a set of eigenfunctions of L_z and $\mathbf{L}^2$. We take the simultaneous eigenfunctions for the three operators to be $Y_{lm}(\theta,\phi)R_l(r)$. Under the assumption that we are dealing with eigenfunctions of the $\mathbf{L}^2$ operator, we have

$$\nabla \to \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2}$$

and the full Schrodinger equation becomes

$$\left[-\frac{\hbar^2}{2m}\Big(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\Big) + V(r) + \frac{l(l+1)\hbar^2}{2mr^2}\right]R_{nl}(r) = ER_{nl}(r)$$

Remark. (Solutions of the above formulation) Imagine solving the equation in the free-particle case, which we know the solution of to be $\exp(ip\cdot x)/(\sqrt{2\pi\hbar})^2$. With the substitution $\rho = kr$ and $k = 2mE/\hbar^2 > 0$, we have

$$\rho^2\frac{d^2R}{d\rho^2} + 2\rho\frac{dR}{d\rho} + (\rho^2 - l(l+1))R = 0$$

which is the spherical Bessel equation, an self-adjoint equation. Substitute $R(\rho) = Z(\rho)/\sqrt{\rho}$ to find

$$\rho^2 Z'' + \rho Z' + \Big(\rho^2 - \Big(l + \frac{1}{2}\Big)^2\Big)Z = 0$$

which is the original Bessel equations. The solutions are given as the Bessel functions $J_{l+1/2}(\rho)$ and the Neumann functions $N_{l+1/2}(\rho)$. Reserving the substitutions, we have the spherical Bessel and spherical Neumann functions $j_l(\rho)$ and $n_l(\rho)$. We can create linear combinations of these functions to obtain spherical Hankel functions, which represent travelling waves. In the limit, we have

$$j_l(\rho) \sim \frac{1}{\rho}\sin\Big(\rho - \frac{l\pi}{2}\Big) \quad n_l(\rho) \sim \frac{1}{\rho}\cos\Big(\rho - \frac{l\pi}{2}\Big)$$

Example. (Spherical well) Now consider the spherical well problem. When $r \geq a$, we have $R_l(r = a) = 0$. Inside the well, we have $j_l(kr)$ and $n_l(kr)$, but we reject the latter as $n_l(kr)$ diverges at the origin. As the wavefunction needs to be continuous at $r = a$, we have

$$j_l(ka) = 0$$

and $ka = x_{nl}$ where x_{nl} denotes the n-th root of $j_l(x)$. We thus find k to be x_{nl}/a and the energy values to be

$$E_{nl} = \frac{\hbar^2}{2m}\Big(\frac{x_{nl}}{a}\Big)^2$$

The last step is normalisation. We impose that

$$\int_0^\infty r^2 dr\,(j_l)^2(Y_{lm})^2 = 1$$

to obtain the coefficients.

Example. (Hydrogen atom) For the Hydrogen atom, we need to substitute the Coulomb potential,

$$V(|\mathbf{r}|) = \frac{1}{4\pi\varepsilon_0}\frac{(-e)Ze}{r}$$

We note that we solve this for negative energy levels, we want bounded motion. Define $\rho = \sqrt{8m(-E)/\hbar^2}r$ and $\lambda = Z\alpha\sqrt{mc^2/2(-E)}$. We then have the equation

$$R'' + \frac{2}{\rho}R' - \frac{l(l+1)}{\rho^2}R + \Big(\frac{\lambda}{\rho} - \frac{1}{4}\Big)R = 0$$

We know that the asymptotic factor must be $\exp(-\rho/2)$, so we take the ansatz $R = \exp(-\rho/2)G(\rho)$ to find

$$G'' - \Big(1 - \frac{2}{\rho}\Big)G' + \Big[\frac{\lambda - 1}{\rho} - \frac{l(l+1)}{\rho^2}\Big]G = 0$$

As $\rho \to 0$, we find $G = \rho^l$ or $G = \rho^{-(l+1)}$. However, as $l \geq 0$, we take the prior, and again set yet another ansatz $R = \exp(-\rho/2)\rho^l H(\rho)$ to find

$$H'' + \Big(\frac{2l+1}{\rho} - 1\Big)H' + \frac{\lambda - l - 1}{\rho}H = 0$$

which follows the form of an Associated Laguerre equation. We can verify that for the Laguerre equations L_{nr}^k satisfy

$$\rho(L_{n_r}^k)'' + (k+1-\rho)(L_{n_r}^k)' + n_r L_{n_r}^k = 0$$

12 Lecture 26 (June 9th)

Remark. Last class we have arrived at the differential equation

$$\rho H'' + (2l+2-\rho)H' + (\lambda - l - 1)H = 0$$

which followed the form of an associated Laguerre equation.

$$\rho(L_{n_r}^k)'' + (k+1-\rho)(L_{n_r}^k)' + n_r L_{n_r}^k = 0$$

Such a differential equation can be solved through the Frobenius method. We note that it is required that $n_r \in \boldsymbol{Z}^+$. We can equate the two equations with $k = 2l+1$ and $\lambda = n = l+1+n_r \geq 1$ ($n \in \boldsymbol{N}$). This n is what we've learned in chemistry as the principle quantum number. With this information, we find the energy levels to be

$$E_n = -\frac{Z^2\alpha^2 mc^2}{2n^2} = -\frac{Z^2}{n^2}(13.6 \text{ eV})$$

In this equation, the mass m is technically the reduced mass,

$$m = \frac{Zm_e m_p}{m_e + Zm_p}$$

The total wavefunction then becomes

$$\psi_{n,l,m} = R_{n,l}(r)Y_{l,m}(\theta,\phi)$$

For a particular n and a corresponding energy level, there are $2n^2$ degeneracies, meaning that there are $2n^2$ states for a single energy level.

Theorem. (Separation of variables for the harmonic oscillator) Consider the Hamiltonian

$$H = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m} + V(x,y,z)$$

We sometimes take the potential to be a summation of component-dependent potentials $V(x,y,z) = V(x) + V(y) + V(z)$. Then, we can take $\psi(x,y,z) = X(x)Y(y)Z(z)$ as a separable solution. Also, take

$$V(x,y,z) = \frac{1}{2}k_x x^2 + \frac{1}{2}k_y y^2 + \frac{1}{2}k_z z^2$$

and we can find the energy levels to be

$$\hbar\omega\left(n_x + n_y + n_z + \frac{3}{2}\right)$$

Notice, how, we can also write the potential energy as $kr^2/2$. Then, we can also do variable separables and obtain a function in the form of

$$\psi(r, \theta, \phi) = R(r)Y(\theta, \phi)$$

We notice how solutions can become very complex when using different coordinate systems.

Definition. We previously noted that the angular momentum can take half-integer values where we denote the values by s. Take $S = 1/2$, and we use the following conventions for the possible kets

$$\left|S = \frac{1}{2}, S_z = \frac{1}{2}\right\rangle = |\uparrow\rangle \qquad \left|S = \frac{1}{2}, S_z = -\frac{1}{2}\right\rangle = |\downarrow\rangle$$

We then see that $\langle\uparrow | \uparrow\rangle = \langle\downarrow | \downarrow\rangle = 1$ and $\langle\uparrow | \downarrow\rangle = 0$. With this information, we can find the matrix representation of $\hat{S}_z$ with respect to the above eigenkets that construct a basis, and we find

$$\hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{\hbar}{2}\sigma_z$$

The eigenkets are named qubits. We now define

$$S_{\pm} = S_x \pm iS_y$$

and seek their matrix representations. We find that

$$S_+ = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad S_- = \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

from which follows that

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{\hbar}{2}\sigma_x \quad \text{and} \quad S_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \frac{\hbar}{2}\sigma_y$$

The Pauli matrices together satisfy the following properties

(i) Hermitian

(ii) $\sigma_x^2 = \sigma_y^2 + \sigma_z^2 = I$ and hence unitary

(iii) $\sigma_i\sigma_j = i\varepsilon_{ijk}\sigma k = -\sigma_j\sigma_i$ where $\{i, j, k\} = \{x, y, z\}$

(iv) $\{\sigma_i, \sigma_j\} = \sigma_i\sigma_j - \sigma_j\sigma_i = \delta_{ij}2I$ which is to say that the Pauli matrices satisfy the Clifford algebra

13 Lecture 27 (June 11th)

Theorem. We try to seek the eigenvectors for S_x and S_y in the basis generated by S_z. The characteristic equation for S_x is

$$\lambda^2 - \left(\frac{\hbar}{2}\right)^2 = 0$$

and $\lambda = \pm\hbar/2$. Let the first eigenvector be denoted as $v = (v_1, v_2)$ we find that $v_1 = v_2$ and from the normalisation condition, $v_1^2 + v_2^2 = 1$ and we find that $v_1 = v_2 = 1/\sqrt{2}$ where choose the sign to be positive by convention. We can also multiply -1 to either v and u, but this would only change the spinor by a phase factor, and as same rays, they would have the same physical meaning.

$$v = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} = |S_x, \uparrow\rangle \quad \text{and} \quad u = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} = |S_x, \downarrow\rangle$$

for eigenvalues $\lambda_u = \hbar/2$ and $\lambda_v = -\hbar/2$ respectively. Similarly, the characteristic equation for S_y is identical with S_x and along with the normalisation condition, we find

$$v = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix} = |S_y, \uparrow\rangle \quad \text{and} \quad u = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix} = |S_y, \downarrow\rangle$$

for eigenvalues $\lambda_v = \hbar/2$ and $\lambda_u = -\hbar/2$ respectively. We can additionally notice that they are perpendicular to each other.

Proposition. We now seek to the spin in an arbitrary direction $\hat{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, the characteristic equation is still $\lambda^2 = n_x^2 + n_y^2 + n_z^2 = 1$. The problem set related to this will definitely be in the test!

Remark. Consider an arbitrary spin state that is normalised. What is the probability that the result is $-\hbar/2$ when it is measured in the $\hat{n}$ direction? We simply expand the state with respect the basis and calculate the square of the coefficients.

$$|\psi\rangle = c_1|\mathbf{S}\cdot\hat{n}, \uparrow\rangle + c_2|\mathbf{S}\cdot\hat{n}, \downarrow\rangle$$

Theorem. We show that there exists an operator that changes the spin state by an angle ϕ.

$$\exp\left(-\frac{i\mathbf{S}\cdot\hat{n}\,\phi}{\hbar}\right)$$

For simplicity, take $\hat{n} = \hat{\mathbf{x}}$.

$$\exp\Big(-\frac{i\sigma_x\phi}{2}\Big) = \sum_{n\in 2\boldsymbol{Z}} \frac{1}{n!}\Big(-\frac{i\phi}{2}\Big)^n(\sigma_x)^n + \sum_{n\in 2\boldsymbol{Z}+1}\Big(-\frac{i\phi}{2}\Big)^n(\sigma_x)^n$$

Which equal to

$$\cos\Big(\frac{\phi}{2}\Big)I - i\sin\Big(\frac{\phi}{2}\Big)\sigma_x = \begin{pmatrix} \cos\frac{\phi}{2} & -i\sin\frac{\phi}{2} \\ -i\sin\frac{\phi}{2} & \cos\frac{\phi}{2} \end{pmatrix}$$

Lets take the $(1,0)$ ket and rotate it by using the above matrix with $\phi = \pi/2$. What we expect is it to lie in S_y. This is true as we find

$$U_{\pi/2}(\hat{\mathbf{x}}) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

We can caluclate to also find that after 360 degrees, the matrix is

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

and after 720 degrees, the matrix is

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

In this sense, spinors are double valued.

Remark. There exists (god given) magnetic moment for electrons. To properly approach this, we require the Dirac equation, where we would apply an operator to the equation and do unrelativistic approximations. We then find

$$\hat{\mathbf{H}} = -\boldsymbol{\mu}\cdot\mathbf{B}(t)$$

with

$$\boldsymbol{\mu} = \frac{q(-e)}{2m_e}\mathbf{S}$$

and $g = 2 \times 1.0011596\ldots$. For orbital angular momentum, $g = 1$. Let try and use this Hamiltonian to solve the equations of motion. What we expect is precessional motion.

Proof. Take

$$|\psi(t)\rangle = \begin{pmatrix} \alpha_\uparrow(t) \\ \alpha_\downarrow(t) \end{pmatrix}$$

and we have

$$\frac{eg\hbar}{4m_e}\boldsymbol{\sigma}\cdot\mathbf{B}(t)\begin{pmatrix} \alpha_\uparrow(t) \\ \alpha_\downarrow(t) \end{pmatrix} = i\hbar\begin{pmatrix} \dot{\alpha}_\uparrow(t) \\ \dot{\alpha}_\downarrow(t) \end{pmatrix}$$

Taking $\mathbf{B} = B_0\hat{\mathbf{z}}$, we simply have the differential equations

$$i\dot{\alpha}_\uparrow(t) = \frac{egB_0}{4m_e}\alpha_\uparrow(t)$$

and

$$i\dot{\alpha}_\downarrow(t) = -\frac{egB_0}{4m_e}\alpha_\downarrow(t)$$

These have simple solutions,

$$\begin{cases} \alpha_\uparrow(t) = \alpha_\uparrow(0)e^{-iw_0t} \\ \alpha_\downarrow(t) = \alpha_\downarrow(0)e^{iw_0t} \end{cases}$$

Finding the expectation values with assuming hat initially the spin was up with $\alpha_\uparrow(0) = \alpha_\downarrow(0) = 1/\sqrt{2}$, we have

$$\langle\psi(t)|\hat{S}_x|\psi(t)\rangle = \frac{\hbar}{2}\frac{1}{\sqrt{2}}(e^{i\omega_0t}, e^{-i\omega_0t})\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}e^{-i\omega_0t}\\ e^{i\omega t}\end{pmatrix} = \frac{\hbar}{4}(e^{2i\omega_0t}+e^{-2i\omega_0t}) = \frac{\hbar}{2}\cos(2\omega_0t)$$

for S_y, we find the same result but with the sine function. □

14 Lecture 28 (June 16th)

Theorem. (Addition of angular momentum) The sum of two angular momentum operators

$$\mathbf{J} = \mathbf{J}_1 \otimes I_2 + I_1 \otimes \mathbf{J}_2$$

must operate both on $|j_2, j_{1z}\rangle$ (the Hilbert space generated by $\mathbf{J}_1$) and $|j_2, j_{2z}$, and therefore acts on the tensor product $|j_1, j_{1z}\rangle \otimes |j_2, j_{2z}\rangle = |j_1, j_{1z}; j_2, j_{2z}$. Note that $[J_{1a}, J_{2b}] = 0$ and that

$$\mathbf{J}^2|j, j_z\rangle = \hbar^2 j(j+1)|j, j_z\rangle$$

with

$$\mathbf{J}_z|j, j_z\rangle = j_z\hbar|j, j_z\rangle$$

We naively take the maximum to be $j_{max} = j_1 + j_2$ and $j_{min} = |j_1 - j_2|$. We now try adding two $S = 1/2$ (Important). We define the total spin as

$$\mathbf{S} = \mathbf{S}_1 \otimes I_2 + I_1 \otimes \mathbf{S}_2$$

with $\mathbf{S}_1$ acting on elements such as $|S_1 = 1/2, S_{1,z}\rangle$ and $\mathbf{S}_2$ acting on elements such as $|S_2 = 1/2, S_{2,z}\rangle$. Then, $\mathbf{S}$ acts on

$$\left|S_1 = \frac{1}{2}, S_{1,z}\right\rangle \otimes \left|S_2 = \frac{1}{2}, S_{1,z}\right\rangle = |S_{1,z}, S_{2,z}\rangle$$

Trying to find the basis of $\mathbf{S}$ starting with $s = 1$ (triplet) we find

$$|s = 1, s_z = 1\rangle = |1/2, 1/2\rangle \otimes |1/2, 1/2\rangle$$

and

$$|s - 1, s_z = -1\rangle = |-1/2, -1/2\rangle$$

what about the middle state with spin 1? We apply $S_- = S_{1,-} + S_{2,-}$ and find

$$|s = 1, s_z = 0\rangle = \frac{1}{\sqrt{2}}\Big(\Big|\frac{1}{2}, -\frac{1}{2}\Big\rangle + \Big| -\frac{1}{2}, \frac{1}{2}\Big\rangle\Big)$$

Now we move on to $S = 0$, where the total spin is 0. We know its going to be a linear combination of $|\uparrow, \downarrow\rangle$ and $|\downarrow, \uparrow\rangle$. As it should be perpendicular with $|1, 0\rangle$, we find

$$|S = 0, S_z = 0\rangle = \frac{1}{\sqrt{2}}\Big(|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle\Big)$$

Does this truely have zero spin ($S = 0$)? Applying $\mathbf{S}^2$ we find

$$\mathbf{S}^2 \frac{1}{\sqrt{2}}\Big(\Big|\frac{1}{2}, -\frac{1}{2}\Big\rangle - \Big| -\frac{1}{2}, \frac{1}{2}\Big\rangle\Big)$$

and using

$$\mathbf{S}^2 = S_x^2 + S_y^2 + S_z^2 + S_z^2 = \frac{1}{2}(S_+S_- + S_-S_+) + S_{1z}^2 + S_{2z}^2 + 2S_{1z}S_{2z}$$

we conclude from

$$\frac{1}{2}S_+S_-(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) = \frac{1}{2}S_+(|\downarrow\downarrow\rangle - |\downarrow\downarrow\rangle) = 0$$

by the same argument, $S_-S_+|0, 0\rangle = 0$ and the remaining calculations on S_z^2 also dissapear. We thus see how indeed, the postulated vector has a spin of zero.