Lecture 3

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- Hermitian Operators
  - So far, we have only considered operators acting on kets:

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

  - If the operator acts on a bra it must act to the left:

$$\langle\epsilon| = \langle\psi|\,A$$

  - However, the bra, $\langle\epsilon|$, is <u>not</u> the bra that corresponds to the ket, $|\phi\rangle = A\,|\psi\rangle$
  - The bra $\langle\phi|$ is found by defining a new operator A^+ that obeys:

$$\langle\phi| = \langle\psi|\,A^+$$

    * A^+ is called the Hermitian adjoint of A. Consider the inner product:

$$\langle\phi|\beta\rangle = \langle\beta|\phi\rangle^*$$
$$\langle\psi|A^+|\beta\rangle = (\langle\beta|A|\psi\rangle)^*$$

    * This relates the matrix elements of A and A^+
    * Therefore, A^+ is found by transposing and complex conjugating the matrix representing A
  - An operator, A, is Hermitian if it is equal to its Hermitian adjoint, A^+
  - If an operator is Hermitian, then its bra, $\langle\psi|\,A$ is equal to the bra $\langle\phi|$ that corresponds to the ket $|\phi\rangle = A\,|\psi\rangle$
    * In quantum mechanics, all operators that correspond to physical observables are Hermitian
  - Hermitian matrices have real eigenvalues, which ensures results of measurements are always real-values

- The eigenvectors of Hermitian matrices comprise a complete set of basis states, which ensures the eigenvectors of any observable are a valid basis

- Projection Operators
  - Recall for a spin-1/2 system we had the identity relation:

$$|+\rangle\langle+| + |-\rangle\langle-| = \mathbb{1}$$

  - We can express this in matrix notation as:

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

  - This gives us the 2x2 identity matrix
  - The individual operators, $|+\rangle\langle+|$ and $|-\rangle\langle-|$, are called projection operators:

$$P_+ = |+\rangle\langle+| = \begin{pmatrix}1 & 0\\0 & 0\end{pmatrix}$$

$$P_- = |-\rangle\langle-| = \begin{pmatrix}0 & 0\\0 & 1\end{pmatrix}$$

  - Thus, for a general state, we may write $P_+ + P_- = \mathbb{1}$
  - From here, we may write:

$$P_+|\psi\rangle = |+\rangle\langle+|\psi\rangle = (\langle+|\psi\rangle)|+\rangle$$
$$P_-|\psi\rangle = |-\rangle\langle-|\psi\rangle = (\langle-|\psi\rangle)|-\rangle$$

  - The effect of the projection operator on a given state is to produce a new, normalized state

$$|\psi'\rangle = P_+|\psi\rangle$$

  - The projection postulate thus becomes:

$$|\psi'\rangle = \frac{P_+|\psi\rangle}{\sqrt{\langle\psi|P_+|\psi\rangle}} = |+\rangle$$

  - This indicates a "collapse" of the quantum state vector

- Measurement
  - In quantum mechanics, one must perform multiple identical measurements on identically prepared systems to infer the probabilities of outcomes

– For example, if one performs N measurements of the projections of $|\psi\rangle$ and obtains $+\hbar/2$ N_+ times, then:

$$\lim_{N\to\infty} \frac{N_+}{N} = |\langle +|\psi\rangle|^2$$

– It is useful to characterize statistical data sets by their mean and standard deviation

$$< S_z >= \frac{\hbar}{2}P_+ + \left(-\frac{\hbar}{2}\right)P_- = \langle\psi|S_z|\psi\rangle = \sum_n a_n P_{a_n}$$

* We may observe that this is the sum of the eigenvalues multiplied by the probability of getting said eigenvalue
* For the spin-1/2 system with $|+\rangle$ we get:

$$< S_z >= \langle +|S_z|+\rangle = \langle +|\hbar/2|+\rangle = \frac{\hbar}{2}\langle +|+\rangle = \frac{\hbar}{2}$$

* Similarly, we may apply $|+\rangle_x$ to observe:

$$< S_z >= {}_x\langle +|S_z|+\rangle_x = {}_x\langle +|\hbar/2|+\rangle_x = \frac{\hbar}{4}(1-1) = 0$$

– It is common to characterize the standard deviation by the root-mean-square:

$$\Delta A = \sqrt{< (A- < A >)^2 >} = \sqrt{< A^2 > - < A >^2}$$

* From the above, it is important to note that in the general case:

$$< A^2 > \neq < A >^2$$

– The square of an operator acts twice on the state:

$$A^2|\psi\rangle = A(A|\psi\rangle)$$

* Similarly, if we consider S_z, we may write:

$$< S_z^2 >= \langle +|S_z^2|+\rangle = \langle +|(\hbar/2)^2|+\rangle = \frac{\hbar^2}{4}$$

* Thus, we may write:

$$\Delta S_z = 0$$

* Now, we check a different orientation:

$${}_x\langle +|S_z^2|+\rangle_x = \frac{\hbar^2}{4}$$

* Thus, we may see:

$$\Delta_x S_z = \frac{h}{2}$$

- Commuting Observables
  - Two incompatible observables may be identified with a commutator:

$$[A, B] = AB - BA$$

  - If $[A, B] = 0$, operators (observables) are said to commute and are compatible
  - Assuming $[A, B] = 0$, then:

$$AB = BA$$

    * Let $|a\rangle$ be an eigenstate of A with eigenvalue a:

$$A|a\rangle = a|a\rangle$$

    * Then we can say:

$$BA|a\rangle = aB|a\rangle$$

    * This can be expanded:

$$AB|a\rangle = A(B|a\rangle) = a|a'\rangle$$

      · Here, we make $B|a\rangle$ an eigenstate of A with eigenvalue a

    * Assuming each eigenvalue has a unique eigenstate, then $B|a\rangle$ must be a scalar multiple of $|a\rangle$

$$B|a\rangle = b|a\rangle$$

    * Thus, we conclude:

$$\text{If } [A, B] = 0, \ A \text{ and } B \text{ have simultaneous sets of eigenstates}$$

    * Conversely, if two operators do not commute, they are incompatible and can not be known simultaneously, like S_z and S_x

- Uncertainty Principle
  - There is an intimate connection between the commutator of two observables and the possible precision of measurements of each:

$$\Delta A \Delta B \geq \frac{1}{2}| < [A, B] > |$$

  - Applying to Stern-Gerlach, we may write:

$$\Delta S_x \Delta S_y \geq \frac{1}{2}| < [S_x, S_y] > |$$

$$\Delta S_x \Delta S_y \geq \frac{\hbar}{2}| < S_z > |$$

* Applying this to $|+\rangle$, we find:

$$\Delta S_x \Delta S_y \geq \left(\frac{\hbar}{2}\right)^2$$

  - This implies that the individual components are both non-zero
  - Therefore, we can not know spin components of either component absolutely
  - As a result, one can not say the spin points in a given direction

- The $\vec{S}$ Operation
  - Let us begin by writing:

$$\vec{S}^2 = S_x^2 + S_y^2 + S_z^2$$

  - It points in no direction in space. We can calculate using matrix notation:

$$\vec{S}^2 = \left(\frac{\hbar}{2}\right)^2 \left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right]$$

$$\vec{S}^2 = \left(\frac{\hbar}{2}\right)^2 [\mathbb{1} + \mathbb{1} + \mathbb{1}]$$

$$\vec{S}^2 = \frac{3\hbar^2}{4}\mathbb{1}$$

  - For any state $|\psi\rangle$ in the Hilbert space $S = 1/2$:

$$\vec{S}^2 |\psi\rangle = \frac{3}{4}\hbar^2 |\psi\rangle$$

  - So, we may conclude:

$$< \vec{S}^2 >= \frac{3}{4}\hbar^2$$

  - This would imply the "length" of the spin vector is:

$$|\vec{S}| = \sqrt{< \vec{S}^2 >} = \sqrt{3}(\hbar/2)$$

  - Thus, this value is greater than the measured component, $\hbar/2$, implying that the spin vector is never fully aligned with any axis

- Spin-1 Systems
  - The Stern-Gerlach experiment produces 3 beams corresponding to z-axis projections $+\hbar$, 0, and $-\hbar$:

$$|1\rangle, |0\rangle, |-1\rangle \Longrightarrow \begin{cases} S_z |1\rangle & = \hbar |1\rangle \\ S_z |0\rangle & = 0\hbar |0\rangle \\ S_z |-1\rangle & = -\hbar |-1\rangle \end{cases}$$

- Recall eigenvectors are unit vectors in their own basis and an operator is always diagonal in its own basis. This gives us:

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad |0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad |-1\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

  * This then gives us:

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

- We can write the x orientation as:

$$|1\rangle_x = \frac{1}{2}|1\rangle + \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{2}|-1\rangle$$
$$|0\rangle_x = \frac{1}{\sqrt{2}}|1\rangle - \frac{1}{\sqrt{2}}|-1\rangle$$
$$|-1\rangle_x = \frac{1}{2}|1\rangle - \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{2}|-1\rangle$$

- We then do the same for the y orientation:

$$|1\rangle_y = \frac{1}{2}|1\rangle + \frac{i}{\sqrt{2}}|0\rangle - \frac{1}{2}|-1\rangle$$
$$|0\rangle_x = \frac{1}{\sqrt{2}}|1\rangle + \frac{1}{\sqrt{2}}|-1\rangle$$
$$|-1\rangle_x = \frac{1}{2}|1\rangle - \frac{i}{\sqrt{2}}|0\rangle - \frac{1}{2}|-1\rangle$$

- The operators can be written as:

$$S_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$
$$S_y = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

- New Labels
  - The allowed values of spin are $S = 1/2, 1, 3/2, 2, \cdots$
  - The number of beams exiting the Stern-Gerlach with such spin is $2S + 1$ with a minimum value of $-\hbar S$ and a maximum value $+\hbar S$

– We label the state $|S_m\rangle$

$$\vec{S}\,|S_m\rangle = S(S+1)\hbar^2\,|S_m\rangle$$
$$S_z\,|S_m\rangle = m\hbar\,|S_m\rangle$$
$$[\vec{S}^2, S_z] = 0$$

  * Note, S_m is the magnetic quantum number

– Schrödinger Equation

  * The time evolution of a quantum system, is determined by the Hamiltonian of the total energy operator $H(t)$ through the Schrödinger equation:

$$i\hbar\frac{d}{dt}\,|\psi(t)\rangle = H(t)\,|\psi(t)\rangle$$

– The Energy Eigenvalue Equation

$$H\,|E_n\rangle = E_n\,|E_n\rangle$$

  * Where E_n represents the only allowed energies of the system
  * Since H represents the energy, it is observable, Hermitian, and therefore, its eigenvalues form a complete basis
  * SInce H is the only operator appearing in the Schrödinger equation, it is convenient to expand the state vectors in terms of the energy eigenstates:

$$|\psi\rangle = \sum_n \langle n(t)|E_n\rangle$$

  * Substituting the expansion into the Schrödinger equation gets us:

$$i\hbar\frac{d}{dt}\sum_n \langle n(t)|E_n\rangle = \sum_n \langle n(t)E_n|E_n\rangle$$
$$\frac{dC_k(t)}{dt} = -i\frac{E_k}{\hbar}C_k(t)$$

  * We see that a possible solution is:

$$C_k(t) = C_o(t)e^{-iE_k/\hbar}$$

    · Each energy has the same form of the time dependence but a different exponent. At time $t = 0$:

$$|\psi(0)\rangle = \sum_n \langle n|E_n\rangle$$

    · And the time evolution of a time-independent Hamiltonian is:

$$|\psi(t)\rangle = \sum_n C_n e^{-iE_n t/\hbar}\,|E_n\rangle$$

$$H\,|E_n\rangle = E_n\,|E_n\rangle$$

- Note that the factor $e^{-iE_nt/\hbar}$ has the form $e^{-i\omega t}$ found in many areas of physics, such that:

$$\omega_n = \frac{E_n}{\hbar} \Rightarrow E_n = \hbar\omega_n$$

- Energy eigenstates are called stationary states
- If the system is in an energy eigenstate, it remains in that state

* The Bohr Frequency
  - The Bohr frequency may be found as:

$$\omega_{21} = \frac{E_2 - E_1}{\hbar}$$