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Theoretical Physics 3

Quantum Theory 2

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Lecture 1

Course notes and audio recordings of the lectures can be found on DUO

Lecture 2

2.1 Vector Spaces

2.1.1 Examples in Vector Spaces

A. Geometric vectors Summing vectors (*only valid for addition of vectors*):

1. If $\underline{v}_1$ and $\underline{v}_2$ are vectors, then $\underline{v}_1 + \underline{v}_2$ is also a vector
   ➤ The plane bounded by $\underline{v}_1$ and $\underline{v}_2$ is a closed vector space under vector addition.
2. $$(\underline{v}_1 + \underline{v}_2) + \underline{v}_3 = \underline{v}_1 + (\underline{v}_2 + \underline{v}_3)$$
3. There is a zero vector $\underline{0}$ (vector of zero length) such that $\underline{v} + \underline{0} = \underline{v}$.
4. Each vector has an inverse $-\underline{v}$ such that $\underline{v} + (-\underline{v}) = \underline{0}$.
5. $$\underline{v}_1 + \underline{v}_2 = \underline{v}_2 + \underline{v}_1$$
6. $\alpha\underline{v}$ is the vector whose length is α times $|\underline{v}|$ in the same direction as $\underline{v}$ for any real α. This is scalar multiplication.
7. $$(\alpha_1 + \alpha_2)\underline{v} = \alpha_1\underline{v} + \alpha_2\underline{v}$$
   $$\alpha(\underline{v}_1 + \underline{v}_2) = \alpha\underline{v}_1 + \alpha\underline{v}_2$$
8. $$(\alpha\beta)\underline{v} = \alpha(\beta\underline{v})$$
9. $$1 \cdot \underline{v} = \underline{v}$$
10. Dot product:
   $$\underline{v}_1 \cdot \underline{v}_2 = |\underline{v}_1||\underline{v}_2| \cos\theta_{12}$$
11. $$\underline{v}_1 \cdot \underline{v}_2 = (\underline{v}_2 \cdot \underline{v}_1)^*$$
12. Linear combinations:
   $$(\alpha\underline{v}_1 + \beta\underline{v}_2) \cdot \underline{w} = \alpha^*(\underline{v}_1 \cdot \underline{w}) + \beta^*(\underline{v}_2 \cdot \underline{w})$$

13.
$$\underline{v} \cdot \underline{v} = |\underline{v}|^2 \geq 0$$

These are the axioms of the inner product. A vector space with inner product $\equiv$ an inner product space

B. 2-component complex column vectors

$$V = \begin{pmatrix} a \\ b \end{pmatrix}$$

where a and b are complex numbers

1. Addition of two vectors:
$$V = \begin{pmatrix} a \\ b \end{pmatrix} \; ; \; W = \begin{pmatrix} a' \\ b' \end{pmatrix}$$
$$V + W = \begin{pmatrix} a + a' \\ b + b' \end{pmatrix}$$

2.
$$(v_1 + v_2) + v_3 = v_1 + (v_2 + v_3)$$

3.
$$\begin{pmatrix} a \\ b \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \end{pmatrix} = \begin{pmatrix} a \\ b \end{pmatrix}$$

4.
$$\begin{pmatrix} a \\ b \end{pmatrix} + \begin{pmatrix} -a \\ -b \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

5.
$$\alpha \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \alpha a \\ \alpha b \end{pmatrix}$$

6. Inner product of v,w is:
$$(v, w) = \begin{pmatrix} a^* & b^* \end{pmatrix} \begin{pmatrix} a' \\ b' \end{pmatrix} = a^* a' + b^* b'$$

C. Functions of x

$$f(x), \psi(x)$$

These functions form a vector space.

1.
$$(f + g)(x) = f(x) + g(x)$$

2.
$$(\alpha f)(x) = \alpha f(x)$$

3. Inner product:
$$(f, g) = \int_{-\infty}^{\infty} f^*(x) g(x) \, dx$$

2.2 Norm of a vector

The norm of a vector is defined as:

$$||v|| = \sqrt{(v, v)}$$

- ➤ Two vectors are said to be orthogonal if $(v, w) = 0$
  - ➥ orthonormal if there are orthogonal and have a unit norm ($||v|| = ||w|| = 1$)

Lecture 3

3.1 Hilbert Spaces

Wave function of a harmonic oscillator:

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$$

Wave function of atomic hydrogen:

$$\int_{-\infty}^{\infty} r^2 dr \int_0^{\pi} \sin\theta \, d\theta \int_0^{2\pi} d\phi \, |\psi(r,\theta,\phi)|^2 = 1$$

- Wave functions must be square-integrable
- The set of all functions forms a vector space
  - The set of all square-integrable functions also forms a vector space, a subset of the above space (a subspace)
  - A subspace is a vector space which is a subset of another vector space
- A square-integrable function refers to using the Leberque integration

Hilbert space: a complete vector space with an inner product, e.g. the vector space of square-integrable functions on $(-\infty, \infty)$. The inner product is:

$$(\phi, \psi) = \int_{-\infty}^{\infty} \phi^*(x)\psi(x) dx$$

3.2 Bases

1. Span of a set of vectors: the set of all linear combinations of these vectors, e.g. the span of

   $$\left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\}$$

   is the set of linear combinations,

   $$a \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + b \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + c \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} a \\ b \\ c \end{pmatrix}$$

   The span of those three vectors is the set of all 3-component column vectors, were $a, b, c \in \mathbb{C}$
2. A set of N vectors is said to be linearly independent if it is not possible to write a vector from that set as a linear combination of the other vectors.

   $$\left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\}$$

is a linearly independent set since it is not possible to find α and β such that

$$\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \alpha \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + \beta \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

Orthogonal vectors are always linearly independent. The dimension of a finite-dimensional vector space is the max number of vectors forming a linearly-independent set. An infinite-dimensional vector space is one in which there is no upper bound on the size of the linearly-independent sets.

Example: Functions of the form $e^{inx}, n \in \mathbb{N}$
These functions form a linearly-independent set since any two such functions are orthogonal.

$$\int_0^{2\pi} \left(e^{inx}\right)^* e^{imx} dx = 0, n \neq m$$

3. A basis is a set of linearly-independent vectors spanning the whole vector space. An orthonormal basis is a basis whose vectors are orthonormal.

Lecture 4

4.1 Operators I

Examples:

1. energy operator $\rightarrow H$
2. angular momentum operator $\rightarrow \underline{L} = L_x\hat{x} + L_y\hat{y} + L_z\hat{z}$
3. linear momentum operator $\rightarrow \underline{p} = -i\hbar\underline{\nabla},\ p_x = -i\hbar\frac{\partial}{\partial x} = -i\hbar\frac{d}{dx}$
4. position operator $\rightarrow x$ (in 1D)

- operators deal with *dynamical variables*
- they transform wavefunctions:

$$p_x e^{-\frac{x^2}{a^2}} = -i\hbar\frac{d}{dx}e^{-\frac{x^2}{a^2}} = 2i\hbar\frac{x}{a^2}e^{-\frac{x^2}{a^2}}$$

- linear operators are ones that act linearly: $A(c_1v_1 + c_2v_2) = c_1Av_1 + c_2Av_2$
- non-linear operators do exist:

$$\begin{aligned} Av &= v||v|| \\ Acv &= cv||cv|| = c|c|v||v|| \\ &= c|c|Av \neq cAv \end{aligned}$$

- many operators are *unbounded*
- identity operator, I such that $Iv = v$

4.2 Using Linear Operators

1. adding operators:
$$(A + B)v = Av + Bv$$
2. multiplying an operator by a scalar:
$$(cA)v = A(cv)$$
3. product of two operators, i.e. act on v with B first then act on the result with A:
$$(AB)v = A(Bv),\ [AB \neq BA]$$
4. invertible operator, an operator which has an inverse: A^{-1}
A^{-1} being such that
$$AA^{-1} = A^{-1}A = I$$

singular operators are defined as non-invertible operators

$$\begin{aligned} (AB)^{-1} &= B^{-1}A^{-1} \\ (A^{-1})^{-1} &= A \end{aligned}$$

5. any operator A has a unique adjoint, $A^\dagger$
   $A^\dagger$ is the operator such that for any v, w

$$
\begin{aligned}
(v, Aw) &= (w, A^\dagger v)^* \\
(AB)^\dagger &= B^\dagger A^\dagger \\
(A^\dagger)^\dagger &= A \\
(A+B)^\dagger &= A^\dagger + B^\dagger \\
(cA)^\dagger &= c^* A^\dagger
\end{aligned}
$$

4.3 Representation by a matrix

For an orthonormal basis: $\{u_1, u_2, \cdots, u_n\}$

$$
\begin{aligned}
(u_i, u_j) = \delta_{ij} &= \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases} \\
v &= c_1 u_1 + c_2 u_2 + \cdots + c_n u_n \\
w &= Av \\
w &= d_1 u_1 + \cdots + d_n u_n \\
\underline{c} &= \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix} \; ; \; \underline{d} = \begin{pmatrix} d_1 \\ d_2 \\ \vdots \\ d_n \end{pmatrix} \\
\underline{d} &= \hat{A}\underline{c} \\
\hat{A} &= \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ \vdots & & & \\ A_{n1} & A_{n2} & \cdots & A_{nn} \end{pmatrix} \\
A_{ij} &= (u_i, Au_j)
\end{aligned}
$$

This matrix represents the operator A in the basis $\{u_1, u_2, \cdots, u_n\}$

Example:

$$
\left\{ \frac{1}{\sqrt{2}}, \sqrt{\frac{3}{2}} x \right\}
$$

is an orthonormal basis in the space of all functions of the form $f(x) = a_0 + a_1 x$

$$
\begin{aligned}
(u_i, u_j) &= \delta_{ij} \\
\int_{-1}^{1} u_i^*(x) u_j(x) \, dx &= \delta_{ij} *
\end{aligned}
$$

<u>Lecture 5</u>

- **Note:** *order of presenting the basis matters, flipping the order of a 2 base basis transverses the matrix*
- For a function, $f = a + bx = c_1 u_1(x) + c_2 u_2(x)$, calculate the constants using the inner product
- One says that the vector space spanned by $u_1(x)$ and $u_2(x)$ is isomorphic to the vector space of 2-component column vectors

5.1 Dirac Notation

$$
\begin{aligned}
u_1(x) &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |1\rangle \\
u_2(x) &= \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |2\rangle \\
f = a + bx &= \begin{pmatrix} a\sqrt{2} \\ b\sqrt{\frac{2}{3}} \end{pmatrix} = |f\rangle
\end{aligned}
$$

- denote inner product of g and f as $(g, f) = \langle g|f\rangle$

$$
\begin{aligned}
\frac{d}{dx} f &= Df = \hat{D}|f\rangle \\
\left(g, \frac{df}{dx}\right) &= \langle g|\hat{D}|f\rangle
\end{aligned}
$$

- The inner product of $c|g\rangle$ and $|f\rangle$ is $c^*\langle g|f\rangle$
- Ket vectors are vectors in their own right, forming a Hilbert space

5.2 Dual Space

- Each state of a quantum system can be described by a vector belonging to a Hilbert space

Lecture 6

6.1 Degenerate Eigenvalues of an Operator

$$
\begin{aligned}
\hat{A}|\psi\rangle &= \lambda|\psi\rangle \\
c|\psi\rangle &= |c\psi\rangle \\
\hat{A}|c\psi\rangle &= \hat{A}c|\psi\rangle \\
&= c\hat{A}|\psi\rangle \\
&= c\lambda|\psi\rangle \\
&= \lambda c|\psi\rangle = \lambda|c\psi\rangle
\end{aligned}
$$

- λ always corresponds to infinitely many different eigenvectors
- It happens that:

$$
\begin{aligned}
\hat{A}|\psi_1\rangle &= \lambda_1|\psi_1\rangle \\
\hat{A}|\psi_2\rangle &= \lambda_1|\psi_2\rangle \\
|\psi_2\rangle &\neq |\psi_1\rangle
\end{aligned}
$$

- i.e., $|\psi_1\rangle$ and $|\psi_2\rangle$ are linearly independent, but correspond to the same eigenvalues
  - If so, λ is said to be degenerate
  - e.g. for hydrogen, the $2s$, $2p_{m=0}$, and $2p_{m=\pm 1}$ states all have the same energy, E_2
- These states are orthogonal, and hence, linearly independent:

$$
\int \psi^*_{nlm}(r, \phi, \theta)\, \psi_{n'l'm'}(r, \phi, \theta)\, d'r = 0
$$

unless $n = n'$, $l = l'$, *and* $m = m'$

- The E_2 eigenvalues of hydrogen are degenerate
- The span of all the eigenvectors belonging to a degenerate eigenvalue is a vector space.

- The degree of degeneracy of that eigenvalue is the dimension of that space.
  - e.g. the degree of degeneracy of E_2 is 4 - "E_2 is 4-fold degenerate"
- If an operator $\hat{A}$ is represented by a matrix, $\underline{\underline{A}}$, then the eigenvalues of $\hat{A}$ are the same as those of $\underline{\underline{A}}$
  - The eigenvectors of $\hat{A}$ are $\iff$ in correspondence with those of the matrix
- Spectrum of an operator: The set of all its eigenvalues (physicist's definition)
  - $\hat{A} - \lambda\hat{I}$
  - $\hat{A}|\psi\rangle = \lambda|\psi\rangle$
- Momentum operator: $p = -i\hbar\frac{d}{dx}$

$$\begin{aligned} p\psi(x) &= \lambda\psi(x) \\ -i\hbar\frac{d\psi}{dx} &= \lambda\psi(x) \\ \psi(x) &= Ce^{i\frac{\lambda}{\hbar}x} \\ \lambda = a + ib \implies e^{i\frac{\lambda}{\hbar}x} &= e^{\frac{1}{\hbar}(ai-b)x} \end{aligned}$$

for any constant C

$$e^{-bx} \to \begin{cases} 0 & fn \to \infty \\ \infty & fn \to -\infty \end{cases}$$

for positive b

- $\psi(x)$ is not square integrable if $b \neq 0$
- If $b = 0$, then $e^{i\frac{a}{\hbar}x}$ remains of modulus 1, but

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = \int_{\infty}^{-\infty} |C|^2 dx$$

this diverges

- None of these eigenfunctions are square-integrable
- p has no eigenfunctions in the Hilbert space of square-integrable functions
- In physics, functions like $e^{\pm ikx}$ where k is real, are also "eigenfunctions" (i.e. pseudo-eigenfunctions or generalised eigenfunctions)

6.2 Dynamical Variables and Operators

- Each state of a quantum system can be represented by a vector belonging to a Hilbert space, $\mathcal{H}$
- With every dynamical variable is associated a linear operator acting in $\mathcal{H}$
  - e.g. position, momentum, angular momentum, spin, energy
  - i.e. physical quantities that may vary in time
- quantities that are constant in time are not dynamical variables
  - e.g. the charge of the electron, etc
  - therefore, they do not correspond to an operator in quantum mechanics
- The only values a dynamical variable can be found to have in a measurement are the eigenvalues of the operator associated with that variable

Suppose that $|\psi\rangle$ represents a state of a quantum system, and $\hat{A}$ represents a dynamical variable:

$$\hat{A}|\psi_n\rangle = \lambda_n|\psi_n\rangle$$

then the probability to find the result λ_n in an experiment is

$$P(\lambda_n) = \frac{|\langle\psi_n|\psi|\rangle|^2}{\langle\psi_n|\psi_n\rangle\langle\psi|\psi\rangle}$$

Usually one takes

$$\begin{aligned} \langle\psi|\psi\rangle &= 1 \\ \& \ \langle\psi_n|\psi_n\rangle &= 1 \\ \implies P(\lambda_n) &= |\langle\psi_n|\psi\rangle|^2 \end{aligned}$$

Lecture 7

1. Experiment
    - ➤ System is prepared in a certain state
    - ➤ measurement
    - ➤ results
2. Theory
    - ➤ state of system is represented by a state vector, $|\psi\rangle$
    - ➤ we have a theoretical description in which what is measured is described in terms of operators associated to dynamical variables
    - ➤ probabilistic "prediction"

7.1 Consequences of the Probability Rule

- ➤ All the predictions of the theory are based on the state vector, $|\psi\rangle$, representing the system
- ➤ All one can say about the state of a quantum system is what can be deduced from the state vector
- ➤ the state vector constrains all the information that can be known about the system
- ➤ $|\phi_n\rangle$ is an eigenvector $\rightarrow \langle\phi_n|\phi_n\rangle \neq 0$
- ➤ the zero vector never represents a quantum state $\rightarrow \langle\psi|\psi\rangle \neq 0$
- ➤ if the probability of a result, λ, is zero, then finding this result is impossible (within the theoretical model used)
    - ➥ if the probability is one, then the result will be obtained with certainty

7.2 The Principle of Superposition

- ➤ if $|\psi_1\rangle$ and $|\psi_2\rangle$ represents a possible state of a system, then any linear combination of $|\psi_1\rangle$ and $|\psi_2\rangle$ also represents a possible state of the system

$$\Psi_{100}(\underline{r},t) = \psi_{100}(\underline{r} \exp\left[-i\left(\frac{E_1 t}{\hbar}\right)\right]$$
$$\Psi_{200}(\underline{r},t) = \psi_{200}(\underline{r} \exp\left[-i\left(\frac{E_2 t}{\hbar}\right)\right]$$
$$\Psi(\underline{r},t) = c_1\Psi_{100} + c_2\Psi_{200} \text{ is also a possible state}$$

If $\langle\phi_n|\phi_n\rangle = 1$, then

$$P(\lambda_n) = \frac{|\langle|\phi_n|\psi\rangle|^2}{\langle\psi|\psi\rangle}$$

- ➤ multiplying the state vector by a non-zero complex number gives the same probability
- ➤ the ket vectors $c|\psi\rangle, c \in \mathbb{C}$ all represent the same state, regardless of the value of c
- ➤ however, a linear combination of state vectors will be different dependent on the value of c for each state vector

7.3 Hermitian Operators

Definition: an operator, $\hat{A}$, is Hermitian if

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

for any $|\psi\rangle$, $|\phi\rangle$

- ➤ the eigenvalues of Hermitian operators are always real
- ➤ the eigenvectors of Hermitian operators corresponding to different eigenvalues are orthogonal
- ➤ matrices representing Hermitian operators are always Hermitian, i.e. equal to their conjugate transpose

Lecture 8

- ➤ An operator $\hat{A}$ is said to be Hermitian if $\langle\phi|\hat{A}|\psi\rangle = \langle\psi|\hat{A}|\phi\rangle^*$ for any $|\psi\rangle$, $|\phi\rangle$ on which $\hat{A}$ may act.

8.1 Proof of the Orthogonality of Eigenvectors

- $\hat{A}$: Hermitian such that
  - $\hat{A}|\psi_1\rangle = \lambda_1|\psi_1\rangle$
  - $\hat{A}|\psi_2\rangle = \lambda_2|\psi_2\rangle$
  - $\lambda_1 \neq \lambda_2$
  - both λ_1 and λ_2 are real since $\hat{A}$ is Hermitian

$$\begin{aligned}
\langle\psi_1|\hat{A}|\psi_2\rangle &= \lambda_2\langle\psi_1|\psi_2\rangle \\
\langle\psi_2|\hat{A}|\psi_1\rangle* &= \lambda_2^*\langle\psi_2|\psi_1\rangle* \\
\langle\psi_2|\hat{A}|\psi_1\rangle &= \lambda_2\langle\psi_2|\psi_1\rangle \\
\langle\psi_2|\hat{A}|\psi_1\rangle &= \lambda_1\langle\psi_2|\psi_1\rangle \\
0 &= \underbrace{(\lambda_1 - \lambda_2)}_{\neq 0}\underbrace{\langle\psi_2|\psi_1\rangle}_{=0}
\end{aligned}$$

- If $\hat{A}$ is a Hermitian operator acting in a finite-dimensional Hilbert space, then it is always possible to form an orthonormal basis of eigenvectors of $\hat{A}$ and this basis is complete.
- A complete set of vectors is a set of vectors spanning the whole space.
  - A basis is always a complete set, by definition.

Example: 1st Workshop

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

- The first matrix above is Hermitian, and the eigenvectors from a complete set.
- The second matrix above is not Hermitian, and the eigenvectors do not form a complete set.

For infinite-dimensional spaces, there are different possibilities: 1. Infinite square well:

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

This acts on $[-a, a]$ such that $\psi(x = \pm a) = 0$ * There are infinitely many eigenvalues (eigenenergies) for this 2. Free particle: Same operator as above on $(-\infty, +\infty)$, acting on a square-integrable function in that bound

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi = E\psi$$

- This has no solution that is square-integrable
- SHM

$$\begin{aligned}
H &= -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2,\ (-\infty, +\infty) \\
H\psi_n &= E\psi_n \\
E_n &= \hbar\omega\left(n + \frac{1}{2}\right) \\
\psi(x) &= \sum_n c_n\psi_n(x)
\end{aligned}$$

8.2 Probability of Obtaining an eigenvalue

$$\begin{aligned}
P_i = |\langle\phi_i|\psi\rangle|^2 &\iff \\
\langle\phi_i|\phi_1\rangle = 1 &= \langle\psi|\psi\rangle\& \\
\hat{A}|\phi_i\rangle &= \lambda_i|\phi_i\rangle
\end{aligned}$$

If λ_i is degenerate:

$$\hat{A}|\psi_n\rangle = \underbrace{\lambda}_{\forall n}|\psi_n\rangle$$

$$\langle\phi_i|\phi_j\rangle = \delta_{ij}$$

Probability of finding λ is:

$$P(\lambda) = \sum_n |\langle\phi_n|\psi\rangle|^2$$

- This is the sum over all the eigenvectors corresponding to λ
- "Observable" - a Hermitian operator with a complete set of eigenvectors

$$P_i(|\psi\rangle) = |\langle\phi_i|\psi\rangle|^2$$

$$P_i(|\phi_j\rangle) = |\langle\phi_i|\phi_j\rangle|^2 = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

- Finding λ_i or λ_j is mutually exclusive:

$$\sum_i P_i(|\psi\rangle) = 1$$

$$\sum_i |\langle\phi_i|\psi\rangle|^2 = 1$$

$$\sum_i \langle\phi_i|\psi\rangle * \langle\phi_i|\psi\rangle = 1$$

$$\sum_i \langle\psi|\phi_i\rangle\langle\phi_i|\psi\rangle = 1$$

- One must have this, or any $|\psi\rangle$

$$\sum_i |\phi_i\rangle\langle\phi_i| = \hat{I}$$

- The is the completeness relation

8.3 Variance of the distribution of probability

$$(\Delta A)^2 = \langle\psi|\hat{A}^2|\psi\rangle - \langle\psi|\hat{A}|\psi\rangle^2$$

Lecture 9

$$(\Delta A)^2(\Delta B)^2 \geq -\frac{1}{4}(\langle\psi|[\hat{A},\hat{B}]|\psi\rangle)^2$$

- system is represented by $|\psi\rangle, \langle\psi|\psi\rangle = 1$
- two dynamical variables, A and B, represented by two observables, $\hat{A}$ and $\hat{B}$
  - these are Hermitian operators with a complete set of eigenvalues

$$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

- the commutator of $\hat{A}$ and $\hat{B}$ if

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

  one would say that $\hat{A}$ and $\hat{B}$ commute, i.e. for any $|\psi\rangle \to [\hat{A},\hat{B}]|\psi\rangle = 0$

$$[\hat{Q},\hat{P}] = i\hbar\hat{I}$$

- $\hat{I}$ is the identity vector and is usually not indicated for simplicity
  - $[\hat{A},\hat{I}] = 0$
- $[\hat{A},\hat{A}] = 0$
- $[\hat{A},\hat{B}] = -[\hat{B},\hat{A}]$

- $[\hat{A}, f(\hat{A})] = 0$, where $f(\hat{A})$ can be any function of $\hat{A}$
- if $[\hat{A}, \hat{B}] = 0$ and $|\phi_n\rangle$ is an eigenvector of $\hat{A}$, then $\hat{B}|\phi_n\rangle$ is also an eigenvector of $\hat{A}$ corresponding to the same eigenvalue.
- Proof:

$$\hat{A}|\phi_n\rangle = \lambda_n|\phi_n\rangle$$
$$\hat{A}\hat{B}|\phi_n\rangle = \hat{B}\hat{A}|\phi_n\rangle = \lambda_n\hat{B}|\phi_n\rangle$$

- If λ_n is not a degenerate eigenvalue of $\hat{A}$, then $\hat{B}|\phi_n\rangle = \mu_n|\phi_n\rangle$
  - $|\phi_n\rangle$ is also an eigenvector of $\hat{B}$
- Proof:
  - If λ_n were degenerate, then (and only then) could one have several linearly independent eigenvectors of $\hat{A}$ all corresponding to λ_n
  - Since we assume that λ_n is not degenerate, $\hat{B}|\phi_n\rangle$ and $|\phi_n\rangle$ cannot be linearly independent, therefore $\hat{B}|\phi_n\rangle = \mu_n|\phi_n\rangle$ for some non-zero value of μ_n
  - If $[\hat{A}, \hat{B}] = 0$, then one can find a basis of the Hilbert space constructed from eigenvectors common to $\hat{A}$ and $\hat{B}$, and reciprocally

Example:
For atomic hydrogen,
- H - Hamiltonian
- $\underline{L}^2$ and L_z
- angular momentum operators

$$[H, \underline{L}^2] = [H, L_z] = [\underline{L}^2, L_z] = 0$$

One can find functions that are eigenfunctions of all these three operators:

$$\begin{aligned}
&\psi_{nlm}(r, \theta, \phi)\\
&H\psi_{nlm} = E_n\psi_{nlm}\\
&\underline{L}^2\psi_{nlm} = \hbar^2 l(l+1)\psi_{nlm}\\
&L_z\psi_{nlm} = \hbar m\psi_{nlm}
\end{aligned}$$

- $H, \underline{L}^2, L_z$ from a "complete set of commuting observables" in the sense that specifying their eigenvalues (e.g. by specifying the corresponding quantum numbers) define their common eigenvectors unambiguously

$$(\Delta A)^2(\Delta B)^2 \geq -\frac{1}{4}(\langle\psi|[\hat{A}, \hat{B}]|\psi\rangle)^2$$

- if $\hat{A}, \hat{B}$ are Hermitian, $[\hat{A}, \hat{B}] = i\hat{C}$ where $\hat{C}$ is Hermitian

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

- the right hand-side is greater than zero
- $(\Delta A)^2$ is the variance of the probability distribution formed by the $P(\lambda_n)$

$$\hat{A}|\phi_n\rangle = \lambda_n|\phi_n\rangle$$
$$\langle\phi_n|\phi_n\rangle = 1$$

Probability of finding λ_n in the measurement is

$$P(\lambda_n) = |\langle\phi_n|\psi\rangle|^2$$

- inside is the probability amplitude for finding λ_n
- See last lecture for generalisation to degenerate eigenvalues

$$\langle\psi|\hat{A}|\psi\rangle = \langle A\rangle$$

This is the expectation value of $\hat{A}$

$$\sum_n \lambda_n P(\lambda_n)$$

- If $|\psi\rangle$ is such that $\hat{A}|\psi\rangle = \lambda|\psi\rangle$, then $\langle\psi|\hat{A}|\psi\rangle = \lambda$

$$
\begin{aligned}
(\Delta A)^2 &= \langle\psi|(\hat{A} - \langle A\rangle\hat{I})^2|\psi\rangle \\
&= \langle\psi|\hat{A}^2|\psi\rangle - \langle\psi|\hat{A}|\psi\rangle^2
\end{aligned}
$$

ΔA is the uncertainty on A

- If we perform a measurement and get $\lambda^{(1)}$ then again and get $\lambda^{(2)}$ etc, after preparing the system to be back in the unmeasured state

$$
\bar{\lambda} = \frac{1}{n}\sum_j \lambda^{(j)}
$$

$$
(\Delta A)^2 = \langle A^2\rangle - \langle A\rangle^2
$$

$$
(\Delta A)^2 \implies \sigma^2 = \frac{1}{n-1}\sum_j(\lambda^{(j)} - \bar{\lambda})^2
$$

Lecture 10

- If $\Delta A = 0$, there is no dispersion
- $\Delta A = 0$ if $|\psi\rangle$ is an eigenvector of $\hat{A}$
- $\hat{A}|\psi\rangle = \lambda|\psi\rangle$

$$
\begin{aligned}
\hat{A}^2|\psi\rangle &= \lambda^2|\psi\rangle = \hat{A}(\hat{A}|\psi\rangle) \\
&= \hat{A}(\lambda|\psi\rangle) - \lambda\hat{A}|\psi\rangle = \lambda^2|\psi\rangle \\
\langle\psi|\hat{A}^2|\psi\rangle - \langle\psi|\hat{A}|\psi\rangle^2 &= \lambda^2\langle\psi|\psi\rangle - (\lambda\langle\psi|\psi\rangle)^2 \\
&= \lambda^2 = \bar{\lambda}^2 = 0
\end{aligned}
$$

- For finite dimensional spaces, if $|\psi\rangle$ is an eigenvector of $\hat{A}$, then $\rangle\psi|[\hat{A},\hat{B}]|\psi\rangle = 0$ too

$$
\begin{aligned}
\langle\psi|\hat{A}\hat{B} - \hat{B}\hat{A}|\psi\rangle &= \lambda^*\langle\psi|\hat{B}|\psi\rangle - \lambda\langle\psi|\hat{B}|\psi\rangle \\
&= (\lambda - \lambda)\langle\psi|\hat{B}|\psi\rangle = 0
\end{aligned}
$$

complex conjugate goes away since $\hat{A}$ is Hermitian

- If $[\hat{A},\hat{B}] = 0$, then it is possible for $(\Delta A)^2(\Delta B)^2 = 0$
- For $\hat{P}$ as the momentum operator,

$$
\begin{aligned}
\hat{P}|\phi\rangle &= p|\phi\rangle \\
-i\hbar\frac{d}{dx}\phi(x) &= p\phi(x) \\
\phi_p(x) &= Ce^{i\frac{px}{\hbar}}
\end{aligned}
$$

not square summable, therefore not an element of the Hilbert space

- For $\hat{Q}$ as the position operator,

$$
Q\phi(x) = x\phi(x) = a\phi(x)
$$

impossible unless $\phi(x) = 0$, which does not qualify as an eigenfunction

- Take $\phi_p(x)$ as generalised eigenfunction of the momentum operator

10.1 Measurement of P

- What is the probability of finding a certain value, p?
- p is distributed continuously, not quantised
- Better to ask for the probability of finding p between p_1 and p_2?

$$
P[(p_1,p_2)] = \int_{p_1}^{p_2} P(p)\,dp
$$

- $P(p)$ is the density of probability, $P(p)\,dp$ is the probability to find a momentum between p and $p + dp$

➤ $P(p)$ has no physical dimensions

➥ those of the inverse of a momentum, so that $P[(p_1, p_2)]$ is a pure number

$$P(p) = \left| \int_{-\infty}^{\infty} \phi_p^*(x)\phi(x)\, dx \right|^2 = \left| C \int_{-\infty}^{\infty} e^{-i\frac{px}{\hbar}} \psi(x)\, dx \right|^2$$

➤ This is the Fourier transform of $\psi(x)$

$$\begin{aligned}
\phi(k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\frac{px}{\hbar}} \psi(x)\, dx \\
\psi(x) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} \phi(k)\, dk \\
&= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} dk \int_{-\infty}^{\infty} e^{-ikx'} \psi(x')\, dx' \\
&= \frac{1}{2\pi} \int_{-\infty}^{\infty} \psi(x)\, dx \int_{-\infty}^{\infty} e^{ik(x-x')} dx
\end{aligned}$$

Lecture 11

➤ Momentum operator: $p = -i\hbar\frac{d}{dx}$

➤ Position operator: $Q = x$

$$\begin{aligned}
P\phi_k(x) &= P\left[Ce^{ikx}\right] = \hbar k \phi_k(x) \\
\phi(k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x) e^{-ikx} dx \\
\psi(x) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{ikx} dk \\
\delta(x - x') &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-x')} dk f(x') \quad = \int_{-\infty}^{\infty} \delta(x - x') f(x)\, dx
\end{aligned}$$

➤ This is true for any function $f(x)$ that is continuous at $x = x'$

$$\begin{aligned}
\delta(x - x') &= \delta(x' - x) \\
\int_{-\infty}^{\infty} P(k)\, dk = 1 &\implies \int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1 \\
P(k) &= |\phi(k)|^2 |C|^2 \\
\phi_k(x) &= Ce^{ikx} \\
|C|^2 \int_{-\infty}^{\infty} dk &\left[\int_{-\infty}^{\infty} \psi(x) e^{-ikx} dx\right]^* \cdot \left[\int_{-\infty}^{\infty} \psi(x') e^{-ikx'} dx'\right] = 1 \\
|C|^2 \int_{-\infty}^{\infty} dx &\int_{-\infty}^{\infty} \psi^*(x)\psi(x') dx' \cdot \int_{-\infty}^{\infty} e^{ik(x-x')} dk = 1 \\
2\pi |C|^2 \int_{-\infty}^{\infty} dx &\int_{-\infty}^{\infty} \psi^*(x)\psi(x')\delta(x - x')\, dx' = 1 \\
2\pi |C|^2 \int_{-\infty}^{\infty} &dx \psi^*(x)\psi(x) = 1 \\
\implies 2\pi |C|^2 &= 1 \to C = \frac{1}{\sqrt{2\pi}}
\end{aligned}$$

➤ The normalised eigenfunctions of P are:

$$\begin{aligned}
\phi_k(x) &= \frac{1}{\sqrt{2\pi}} e^{ikx} \\
\phi_p(x) &= \frac{1}{\sqrt{2\pi\hbar}} e^{ip\frac{x}{\hbar}}
\end{aligned}$$

- Orthonormality condition here is

$$\int_{-\infty}^{\infty} \phi_k^*(x)\phi_{k'}(x)\,dx = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i(k-k')x}dx = \delta(k'-k)$$
$$\int_{-\infty}^{\infty} \phi_n(x)\phi_{n'}(x)\,dx = \delta_{nn'}$$

11.1 Eigenfunctions of the position operator

$$Q\psi(x) = x\psi(x)$$

An eigenfunction of Q would be such that

$$Q\phi_q(x) \equiv q\phi_k(x) \equiv x\phi_k(x)$$

Finally, one can take:

$$\begin{aligned}
\phi_k(x) &= \delta(x-q) \\
P[(q_1,q_2)] &= \int_{q_1}^{q_2} P(q)\,dq \\
P(q) &= \left| \int_{-\infty}^{\infty} \phi_q^*(x)\psi(x)\,dx \right|^2 \\
&= \left| \int_{-\infty}^{\infty} \delta(q-x)\psi(x)\,dx \right|^2 \\
&= |\psi(q)|^2
\end{aligned}$$

This is the Born Rule

- Normalisation:

$$\int_{-\infty}^{\infty} \delta^*(x-q)\delta(x-q')\,dx = \delta(q-q')$$

- Discrete case: $|\psi\rangle = \sum_n c_n|\phi_n\rangle$ if $\{|\phi_n\rangle\}$ is an orthonormal basis

$$\begin{aligned}
c_n &= \langle\phi_n|\psi\rangle \\
\psi(x) &= \int_{-\infty}^{\infty} \phi(p)\phi_p(x)\,dp,\;\; \phi(p) = \langle p|\psi\rangle \\
\hat{Q}|x\rangle &= x|x\rangle \\
\hat{p}|p\rangle &= p|p\rangle \\
\psi(x) &= \langle x|\psi\rangle
\end{aligned}$$

- $\psi(x) = \langle x|\psi\rangle$ - wave function in position representation in position space
- $\phi(p) = \langle p|\psi\rangle$ - wave function in the momentum representation in momentum space

The last two statements are equivalent

$$|\psi\rangle \leftrightarrow \psi(x)$$
$$|x\rangle \leftrightarrow \begin{pmatrix} a \\ b \end{pmatrix}$$
$$|\psi\rangle \leftrightarrow \phi(p)$$
$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ip\frac{x}{\hbar}}$$
$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{-ix\frac{p}{\hbar}}$$
$$\hat{Q} \leftrightarrow x$$
$$\hat{p} \leftrightarrow -i\hbar\frac{d}{dx}$$
$$\hat{p} \leftrightarrow p$$
$$\hat{Q} \leftrightarrow -i\hbar\frac{d}{dp}$$

In 3D position representation:

$$P_x = -i\hbar\frac{\partial}{\partial x}$$
$$P_y = -i\hbar\frac{\partial}{\partial y}$$
$$P_z = -i\hbar\frac{\partial}{\partial z}$$
$$[x, P_x] = [y, P_y] = [z, P_z] = i\hbar$$
$$[x, y] = [x, z] = [y, z] = 0$$
$$[x, P_y] = [x, P_z] = \cdots = 0$$
$$[P_x, P_y] = [P_x, P_y] = 0$$
$$[x, P_y]\psi(x, y, z) = -i\hbar\left[x\frac{\partial}{\partial y}\psi - \frac{\partial}{\partial y}x\psi\right] = 0$$
$$\underline{P} = P_x\hat{x} + P_y\hat{y} + P_z\hat{z}$$
$$\underline{P}\phi_{\underline{p}}(\underline{r}) = \underline{P}\phi_{\underline{p}}(\underline{r})$$
$$\underline{p} = \hbar\underline{k}$$
$$\phi_{\underline{p}}(\underline{r}) = \frac{1}{\sqrt{2\pi\hbar}} e^{i\underline{p}\cdot\frac{\underline{r}}{\hbar}}$$
$$\phi_{\underline{k}}(\underline{r}) = \frac{1}{\sqrt{2\pi}} e^{i\hbar\underline{r}}$$
$$\int \phi_k^*(\underline{r})\phi_{k'}(\underline{r})\, d^3r = \delta^3(\underline{k} - \underline{k}') = \delta(k_x - k_x')\delta(k_y - k_y')\delta(k_z - k_z')$$

<u>Lecture 12</u>

- ➤ Infinite square well:
  - ➥ The Hamiltonian has infinite many discrete energy levels
- ➤ Linear harmonic oscillator:
  - ➥ Also has infinite many discrete energy levels
- ➤ Free particle in 1D:
  - ➥ continuum of energy levels, $0 < E < \infty$

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

- atom of hydrogen
  - infinitely many discrete energy levels, corresponding to bound states
  - and a continuum of energy levels corresponding to unbound states
  - $-13.6\,eV = T + V$
  - r must be such that $-13.6\,eV > V(r)$
  - an electron with positive energy is in an unbound state
- in general, we have two classes - discrete and bound

1. discrete energy levels:
$$H\phi_j = E_j\phi_j$$
$$\int \phi_i^*\phi_j d^3r = \delta_{ij}$$
2. continuum of energy levels
$$H\phi_{\underline{k}} = E_{\underline{k}}\phi_{\underline{k}}$$
$$\int \phi_{\underline{k}}^*(\underline{r})\phi_{\underline{k}'}\, d^3r = \delta(\underline{k} - \underline{k}')$$
$$\int \phi_i(\underline{r})\phi_{\underline{k}}(\underline{r})\, d^3r = 0$$

- A complete set of eigenfunctions of H necessarily include a continuum eigenfunctions if H has a continuous spectrum:
$$\psi(\underline{r}) = \sum_j c_j\phi_j(\underline{r}) + \int c_{\underline{k}}\phi_{\underline{k}}(\underline{r})\, d^3k$$
- Since the ϕ_j and $\phi_{\underline{k}}$ are orthonormal
$$c_j = \int \phi_j^*(\underline{r}')\psi(\underline{r}')\, d^3r'$$
$$c_{\underline{k}} = \int \phi_{\underline{k}}^*(\underline{r})\psi(\underline{r}')\, d^3r'$$
$$\psi(\underline{r}) = \int d^3r' \underbrace{\left[\sum_j \phi_j(\underline{r})\phi_j^*(\underline{r}') + \int d^3k\phi_{\underline{k}}(\underline{r})\phi_{\underline{k}}(\underline{r}')\right]}_{=\delta(\underline{r}-\underline{r}')}\psi(\underline{r})$$
- Must be true for any $\underline{r}$, and any ψ
- completeness relation from lecture 8
- In Dirac notation:
$$\langle\underline{r}|\sum_j|\phi_j\rangle\langle\phi_j| + \int d^3k|\phi_{\underline{k}}\rangle\langle\phi_{\underline{k}}| = \hat{I}|\underline{r}'\rangle|\phi_j\rangle\langle\phi_j|\psi\rangle$$
- In position representation:
$$\langle\underline{r}|\phi_j\rangle = \phi_j(\underline{r}) = \rangle\phi_j|\underline{r}\rangle^*$$
$$\langle\phi_j|\underline{r}'\rangle = \phi_j^*(\underline{r}')$$
$$\langle\underline{r}|\hat{I}|\underline{r}'\rangle = \delta(\underline{r} - \underline{r}')$$
- About bra vectors
$$|A\psi\rangle = \hat{A}|\psi\rangle$$
$$\langle A\psi| = \langle\psi|\hat{A}^\dagger,\ \langle A\psi|\phi\rangle = \langle\psi|\hat{A}^\dagger|\phi\rangle$$
$$\langle A\psi|\phi\rangle = \langle\phi|A\psi\rangle^* = \langle\phi|\hat{A}|\psi\rangle^* = \langle\psi|\hat{A}^\dagger|\phi\rangle$$

12.1 Unitary Transformations

- 2 orientations for $2p_m = 0$

- Relate the two by:

$$|\psi'\rangle = \hat{R}_x(\theta)|\psi\rangle$$
$$|\phi'\rangle = \hat{R}_x(\theta)|\phi\rangle$$
$$\langle\phi'|\psi'\rangle = \langle\phi|\psi\rangle$$

- The transformation is an isometry
- In fact, it is also a unitary transformation

Lecture 13

13.1 Unitary Operators

- If $\hat{A}^\dagger = \hat{U}^{-1}$, then $\hat{U}$ is a unitary operator
  - $\hat{U}^\dagger\hat{U} = \hat{I} = \hat{U}\hat{U}^\dagger$
  - $\hat{U}^{-1}\hat{U} = \hat{I} = \hat{U}\hat{U}^{-1}$
- $\hat{U}$ is the same for all vectors of the Hilbert space

$$|\psi'\rangle = \hat{U}|\psi\rangle$$
$$|\psi\rangle = \hat{U}^{-1}|\psi'\rangle = \hat{U}^\dagger|\psi'\rangle$$
$$|\phi'\rangle = \hat{U}|\phi\rangle$$
$$|\eta\rangle = \hat{A}|\psi\rangle$$
$$|\eta'\rangle = \hat{U}|eta\rangle = \hat{U}\hat{A}|\psi\rangle = \hat{U}\hat{A}\hat{U}^\dagger|\psi'\rangle$$
$$|\eta'\rangle = \hat{A}'|\psi'\rangle,\ \ \hat{A}' = \hat{U}\hat{A}\hat{U}^\dagger$$

- Line four and seven are of the same form - but latter is written in terms of the transformed vectors and operators.
- $\hat{U}$ transforms:
  - vectors $|\psi\rangle$ into $\hat{U}|\psi\rangle$
  - operators $\hat{A}$ into $\hat{U}\hat{A}\hat{U}^\dagger$
- $\hat{A}' = \hat{U}\hat{A}\hat{U}^\dagger$ has all the same properties of untransformed operator $\hat{A}$
- If $\hat{A}$ is Hermitian, then $\hat{A}'$ is also Hermitian
- If $\hat{A} = \alpha\hat{B} + \beta\hat{C}\hat{D}$, then $\hat{A}' = \alpha\hat{B}' + \beta\hat{C}'\hat{D}'$
- Proof:

$$\hat{A} = \alpha\hat{B} + \beta\hat{C}\hat{D}$$
$$\hat{U}\hat{A}\hat{U}^\dagger = \alpha\hat{U}\hat{B}\hat{U}^\dagger + \beta\hat{U}\hat{C}\hat{I}\hat{D}\hat{U}^\dagger$$
$$\hat{A}' = \alpha\hat{B}' + \beta\hat{C}'\hat{D}'$$

- $[\hat{A}, \hat{B}] = [\hat{A}', \hat{B}']$
- $\hat{A}$ and $\hat{A}'$ have the same eigenvalues
- $\langle\phi|\hat{A}|\psi\rangle = \langle\phi'|\hat{A}'|\psi'\rangle$ for any $|\psi\rangle, |\phi\rangle$
- In particular, $\langle\phi|\psi\rangle = \langle\phi'|\psi'\rangle$
  - inner products are not changed by unitary transformations
- Proof:

$$\begin{aligned}|\psi'\rangle &= \hat{U}|\psi\rangle\\ |\phi'\rangle &= \hat{U}|\phi\rangle\\ \implies \langle\phi'| &= \langle\phi|\hat{U}^\dagger\\ \implies \langle\phi'|\psi'\rangle &= \langle\phi|\hat{U}^\dagger\hat{U}|\psi\rangle\\ &= \langle\phi|\psi\rangle\end{aligned}$$

- In particular, unitary transformations do not change the norm of the vector: $\langle\psi|\psi\rangle = \langle\psi'|\psi'\rangle$

13.2 Time evolution of quantum systems

➤ Time-dependent Schrodinger equation:

$$
\begin{aligned}
i\hbar\frac{d}{dt}|\Psi(t)\rangle &= \hat{H}|\Psi(t)\rangle \\
|\Psi(t)\rangle &= \hat{U}(t,t_0)|\Psi(t_0)\rangle \\
\hat{U}(t,t_0) &= \hat{U}(t,t_1)\hat{U}(t_1,t_0) \\
\hat{U}^\dagger(t,t_0) &= \hat{U}^{-1}(t,t_0) = \hat{U}(t_0,t) \\
\hat{U}(t_0,t_0) &= \hat{I} = \hat{U}(t_0,t)\hat{U}(t,t_0) \\
\implies i\hbar\frac{d}{dt}\hat{U}(t,t_0) &= \hat{H}\hat{U}(t,t_0)
\end{aligned}
$$

➤ $\hat{U}(t,t_0)$ is the time-evolution operator
   ➥ it is unitary
➤ If $\hat{H}$ is time-independent, then

$$
\begin{aligned}
\hat{U}(t,t_0) &= \exp\left[\frac{-i\hat{H}(t-t_0)}{\hbar}\right] \\
e^{\hat{A}} &= \hat{I} + \hat{A} + \frac{1}{2!}\hat{A}^2 + \frac{1}{3!}\hat{A}^3 + \cdots
\end{aligned}
$$

➤ The exponential of an operator is the Taylor expansion of that operator

13.3 Expectation values of observables

$$
\begin{aligned}
\langle\hat{A}(t)\rangle &= \langle\Psi(t)|\hat{A}|\Psi(t)\rangle \\
&= \langle\Psi(t_0)|\underbrace{\hat{U}^\dagger(t,t_0)\hat{A}\hat{U}(t,t_0)}_{\hat{A}_H(t)}|\Psi(t_0)\rangle \\
\hat{A}_H(t) &= \hat{U}^\dagger(t,t_0)\hat{A}\hat{U}(t,t_0) \\
&= \hat{U}(t_0,t)\hat{A}\hat{U}^\dagger(t_0,t) \\
\langle\hat{A}(t)\rangle &= \langle\Psi(t_0)|\hat{A}_H(t)|\Psi(t_0)\rangle
\end{aligned}
$$

1. State vector changes in time, $\hat{A}$ doesn't - Schrodinger picture
2. State vectors do not change in time, $\hat{A}_H(t)$ does - Heisenberg picture

➤ These two formulations are completely equivalent
➤ Heisenberg equation of motion:

$$
i\hbar\frac{d\hat{A}_H(t)}{dt} = [\hat{A}_H,\hat{H}] = [\hat{A},\hat{H}]
$$

if $\hat{A}$ is time-independent.

Lecture 14

$$
\begin{aligned}
\hat{U}^\dagger &= \hat{U}^{-1} \\
|\psi'\rangle &= \hat{U}|\psi\rangle \\
\hat{A}' &= \hat{U}\hat{A}\hat{U}^\dagger
\end{aligned}
$$

➤ The eigenvalues of a unitary operator are real or complex numbers of modulus 1
➤ The eigenvectors of a unitary operator corresponding to different eigenvalues are orthogonal to each other

$$
\begin{aligned}
\langle A\rangle(t) &= \langle\Psi(t)|\hat{A}|\Psi(t)\rangle \\
&= \langle\Psi(t_0)|\hat{A}_H(t)|\Psi(t_0)\rangle \\
\hat{A}_H(t) &= \hat{U}(t_0,t)\hat{A}\hat{U}^\dagger(t_0,t) \\
i\hbar\frac{d\hat{A}_H}{d}t &= [\hat{A}_H,\hat{H}_H] = \hat{U}(t_0,t)[\hat{A},\hat{H}]\hat{U}^\dagger(t_0,t)
\end{aligned}
$$

- If $[\hat{A},\hat{H}]=0$, then $\hat{A}_H$ is constant in time
  - $\langle A\rangle(t)$ is also constant for any $|\Psi\rangle$
  - A is a "constant of motion"

$$
\begin{aligned}
|\psi'\rangle &= \hat{R}_x(\theta)|\psi\rangle \\
\langle\psi'|H|\psi'\rangle &= \langle\psi|\hat{H}|\psi\rangle \\
\langle\psi|\hat{R}_x(-\theta)\hat{H}\hat{R}_x(\theta)|\psi\rangle &= \langle\psi|\hat{H}|\psi\rangle \\
\hat{R}_x^\dagger(theta) &= \hat{R}_x^{-1}(\theta = \hat{R}_x(-\theta) \\
\langle\psi'| &= \langle\psi|\hat{R}_x^\dagger(\theta) \\
&= \langle\psi|\hat{R}_x(-\theta)
\end{aligned}
$$

- Now look at the limit when $\theta\to\epsilon$, where ϵ is near zero

$$
\begin{aligned}
\hat{R}_x(\pm\epsilon) &= \hat{I} \mp i\epsilon\frac{\hat{J}_x}{\hbar} \\
\langle\psi|\left(\hat{I}+i\frac{\epsilon}{\hbar}\hat{J}_x\right)\hat{H}\left(\hat{I}-\frac{i\epsilon}{\hbar}\hat{J}_x\right)|\psi\rangle &= \langle\psi|\hat{H}|\psi\rangle \\
\langle\psi|\hat{H}|\psi\rangle + \langle\psi|\frac{i\epsilon}{\hbar}\hat{J}_x\hat{H}|\psi\rangle + \langle\psi|\frac{-i\epsilon}{\hbar}\hat{H}\hat{J}_x|\psi\rangle &= \langle\psi|\hat{H}|\psi\rangle + \frac{i\epsilon}{\hbar}\langle\psi|[\hat{J}_x,\hat{H}]|\psi\rangle \\
&= \langle\psi|\hat{H}|\psi\rangle \text{ for any } \psi \\
\implies [\hat{J}_x,\hat{H}] &= 0
\end{aligned}
$$

- The requirement that the state of the atom is invariant under a rotation means that $\underline{J}$ is a constant

14.1 unitary transformations and change of bases

- dimension of the Hilbert space, N
- Consider two different orthonormal bases for that space:

$$
\begin{aligned}
&\{|\phi_1\rangle,|\phi_2\rangle,\cdots,|\phi_N\rangle\} \\
&\{|\psi_1\rangle,|\psi_2\rangle,\cdots,|\psi_N\rangle\} \\
&\langle\phi_i|\phi_j\rangle = \delta_{ij},\ \langle\psi_i,\psi_j\rangle = \delta_{ij}\sum_{i=1}^N|\phi_i\rangle\langle\phi_i| \quad = \hat{I},\ \sum_{i=1}^N|\psi_i\rangle\langle\psi_i| = \hat{I}
\end{aligned}
$$

- The last line is the Completeness relation
- An operator $\hat{A}$ is represented by a matrix $\underline{\underline{A}}$ in the $\{|\phi\rangle\}$ basis, $\underline{\underline{A}}'$ in the $\{|\psi\rangle\}$ basis

$$
\begin{aligned}
A_{ij} &= \langle\phi_i|\hat{A}|\phi_j\rangle \\
A'_{ij} &= \langle\psi_i|\hat{A} \\
psi_j\rangle
\end{aligned}
$$

- Because the $\{|\phi\rangle\}$ vectors are a basis, one can always write each of the $|\psi_j\rangle$ vectors as a linear combination of the $|\phi_i\rangle$ vectors:

$$
\begin{aligned}
|\psi_j\rangle &= \sum_i U_{ji}^* |\phi_i\rangle \\
U_{ji}^\dagger &= \langle\phi_i|\psi_j\rangle = \langle\psi_j|\phi_i\rangle^* \\
U_{ji} &= \langle\psi_j|\phi_i\rangle \\
\underline{\underline{U}} &= \begin{pmatrix} U_{11} & U_{12} & \cdots & U_{1N} \\ \vdots & \ddots & & \vdots \\ U_{N1} & \cdots & \cdots & U_{NN} \end{pmatrix} \\
\underline{\underline{U}}\underline{\underline{U}}^\dagger &= \underline{\underline{I}} \\
(\underline{\underline{U}}\underline{\underline{U}}^\dagger)_{ij} &= \sum_k U_{ik} U_{kj}^\dagger \\
&= \sum_k \langle\psi_i|\phi_k\rangle\langle\phi_k|\psi_j\rangle \\
&= \langle\psi| \underbrace{\sum_k |\phi_k\rangle\langle\phi_k|}_{\hat{I}} |\psi_j\rangle \\
&= \langle\psi_i|\psi_j\rangle = \delta_{ij}
\end{aligned}
$$

$$
\begin{aligned}
\hat{A}' &= \hat{U}\hat{A}\hat{U}^\dagger & |\chi\rangle &= \sum_i c_i |\phi_i\rangle \\
\hat{c}' &= \hat{U}\hat{c} & &= \sum_i c_i' |\psi_i\rangle
\end{aligned}
$$

Lecture 15

15.1 Spectral Decomposition

Recall that $\sum_n |\phi_n\rangle\langle\phi_n| + \int d^3k |\phi_{\underline{k}}\rangle\langle\phi_{\underline{k}}| = \hat{I}$ if and only if $\{|\phi_n, |\phi_{\underline{k}}\rangle\}$ is complete.

$$
\begin{aligned}
\hat{A}|\phi_n\rangle &= a_n|\phi_n\rangle & \langle\phi_i|\phi_j\rangle &= \delta_{ij} \\
\hat{A}|\phi_{\underline{k}}\rangle &= a_{\underline{k}}|\phi_{\underline{k}}\rangle & \langle\phi_{\underline{k}}|\phi_{\underline{k}'}\rangle &= \delta(\underline{k} - \underline{k}')
\end{aligned}
$$

- ➤ $\hat{A}$ is a Hermitian operator

$$
\begin{aligned}
\hat{A} &= \hat{A}\hat{I} \\
&= \sum_n \hat{A}|\phi_n\rangle\langle\phi_n| + \int d^3k \hat{A}|\phi_{\underline{k}}\rangle\langle\phi_{\underline{k}}| \\
&= \sum_n a_n|\phi_n\rangle\langle\phi_n| + \int d^3k a_{\underline{k}}|\phi_{\underline{k}}\rangle\langle\phi_{\underline{k}}|
\end{aligned}
$$

- ➤ This is the spectral decomposition of $\hat{A}$

15.2 Projectors

For example,

$$
\begin{aligned}
\hat{\mathcal{P}}_\phi &= |\phi\rangle\langle\phi| \text{ with } \langle\phi|\phi\rangle = 1 \\
\hat{\mathcal{P}}_\phi|\psi\rangle &= |\phi\rangle\langle\phi|\psi\rangle = \langle\phi|\psi\rangle|\phi\rangle
\end{aligned}
$$

In position representation:

$$
\begin{aligned}
\mathcal{P}_\phi\psi(\underline{r}) &= \left[\int \phi^*(\underline{r}')\psi(\underline{r}')d^3r\right]\phi(\underline{r}) \\
\mathcal{P}_\phi &\equiv \phi^*(\underline{r}')\phi(\underline{r}')
\end{aligned}
$$

in the sense that when $\mathcal{P}_\phi$ acts on a wave function, $\psi(\underline{r})$, the result is as above

$$\begin{aligned}
\hat{\mathcal{P}}_\phi &= |\phi\rangle\langle\phi| \\
\hat{\mathcal{P}}_\phi^2 &= \hat{\mathcal{P}}_\phi\hat{\mathcal{P}}_\phi = |\phi\rangle\langle\phi|\phi\rangle\langle\phi| \\
&= \phi\rangle\langle\phi| = \hat{\mathcal{P}}_\phi
\end{aligned}$$

- $\hat{\mathcal{P}}_\phi$ is idempotent
  - operators $\hat{A}$ such that $\hat{A}^2 = \hat{A}$ are said to be idempotent
- $\hat{\mathcal{P}}_\phi$ is also Hermitian:

$$\begin{aligned}
\langle\psi'|\hat{\mathcal{P}}_\phi|\psi\rangle &= \langle\psi|\hat{\mathcal{P}}_\phi|\psi'\rangle^* \\
&= \langle\psi'|\phi\rangle\langle\phi|\psi\rangle \\
&= \langle\phi|\psi\rangle\langle\psi'|\phi\rangle \\
&= \langle\psi|\phi\rangle^*\langle\phi|\phi'\rangle^* \\
&= [\langle\psi|\phi\rangle\langle\phi|\psi'\rangle]^*
\end{aligned}$$

More generally, any operator which is both idempotent and Hermitian is a projector. Consider a vector, $\underline{v}$ in 3D space:

- $\underline{v} = v_x\hat{x} + v_y\hat{y} + v_z\hat{z}$
- $\underline{w} = v_x\hat{x} + v_y\hat{y}$ - this is the projection of $\underline{v}$ in the x-y plane
- $\underline{w} = (\hat{x}\hat{x} + \hat{y}\hat{y}) \cdot \underline{v} = \hat{x} \cdot \underline{v}\hat{x} + \hat{y} \cdot \underline{v}\hat{y}$
- $(\hat{x} \cdot \underline{v}$ is the same as $|\hat{x}\rangle\langle\hat{x}|\underline{v}\rangle$
- The projection in the plane is affected by $|\hat{x}\rangle\langle\hat{x} + |\hat{y}\rangle\langle\hat{y}|$
- If $|\phi\rangle$ and $|\psi\rangle$ are linearly independent, $\langle\phi|\psi\rangle = 0, \langle\phi|\phi\rangle = \langle\psi|\psi\rangle = 1$
- $|\psi\rangle\langle\phi| + |\psi\rangle\langle\psi|$ projectors in the subspace spanned by $|\phi\rangle$ and $|\psi\rangle$

$$\sum_n |\phi_n\rangle\langle\phi_n| + \int d^3k|\phi_{\underline{k}}\rangle\langle\phi_{\underline{k}}| = \hat{I}$$

- $\hat{\mathcal{P}}_\phi = |\phi\rangle\langle\phi|$ is Hermitian
- $|\langle\phi|\psi\rangle|^2$ is the probability of finding the system in a state $|\phi\rangle$ if it was in the state $|\psi\rangle$ before measurement
- If $|\eta\rangle$ is an eigenvector of $\hat{\mathcal{P}}_\phi$ with eigenvalue η:

$$\begin{aligned}
\hat{\mathcal{P}}_\phi|\eta\rangle &= \eta|\eta\rangle \\
|\phi\rangle\langle\phi|\eta\rangle &= \eta|\eta\rangle \\
\langle\phi|\eta\rangle|\phi\rangle &= \eta|\eta\rangle \\
\implies |\phi\rangle &= |\eta\rangle,\ \eta = 0, \langle\phi|\eta\rangle = 0, 1
\end{aligned}$$

The eigenvalues of $\hat{\mathcal{P}}_\phi$ are 0 and 1

- For $\eta = 1$ - $|\eta\rangle = |\phi\rangle$
- For $\eta = 0$ - $|\eta\rangle$ can be any vector orthogonal to $|\phi\rangle$
- Observable here - $\hat{\mathcal{P}}_\phi$
- Possible outcomes - $\eta = 0, 1$
- Probability of finding $\eta = 1$ - $|\langle\phi|\psi\rangle|^2$

15.3 Revision of ladder operator

- $\hat{a}_- = \hat{a}$, and $\hat{a}_+ = \hat{a}^\dagger$
- subscript with dimension being used in - x,y,z

$$\begin{aligned}
[\hat{a}_i, \hat{a}_i^\dagger] &= 1 \\
[\hat{a}_i, \hat{a}_j^\dagger] &= 0
\end{aligned}$$

Lecture 16

16.1 Comments on Homework

- $[\hat{H}.\hat{U}(t,t_0)] = 0$ because if $\hat{H}$ is time-independent, $\hat{U}(t,t_0) = \exp[-i\hat{H}(t-t_0)/\hbar]$

16.2 Operators and Spin States

- Consider operators belonging to orthogonal directions, i.e. ladder operators
- We then define the Hamiltonian, $\hat{H} = \hbar\omega(\hat{a}_x^\dagger \hat{a} + \frac{1}{2})$
- This then leads to $E_n = \hbar\omega(n+\frac{1}{2}), n = 0,1,2 \implies \hat{a}_x|\phi_n\rangle = \sqrt{n}|\phi_{n-1}\rangle, \hat{a}_x|\phi_0\rangle = 0$
- $\hat{a}_x^\dagger|\phi_n\rangle = \sqrt{n+1}|\phi_{n+1}$

16.3 Angular Momentum

- The orbital angular momentum operator is $\underline{L} = \hat{L}_x\hat{i} + \hat{L}_y\hat{j} + \hat{L}_z\hat{k}$

$$\underline{L} = \underline{r}\times\underline{p},\ \underline{r} = \hat{x}\hat{i} + \hat{y}\hat{j} + \hat{z}\hat{k},\ \hat{p} = \hat{p}_x\hat{i} + \hat{p}_y\hat{j} + \hat{p}_z\hat{k}$$

$$\underline{L} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \hat{x} & \hat{y} & \hat{z} \\ \hat{p}_x & \hat{p}_y & \hat{p}_z \end{vmatrix}$$

$$\begin{aligned}
&\implies \hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y \\
&\implies \hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z \\
&\implies \hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x \\
&\implies \hat{L}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = -i\hbar\frac{\partial}{\partial\phi}
\end{aligned}$$

- Another example is the spin operator, i.e. $\underline{s} = \hat{s}_x\hat{i} + \hat{s}_y\hat{j} + \hat{s}_z\hat{k}$
- An operator $\underline{J}$ is an angular momentum operator if $\hat{J}_x, \hat{J}_y, \hat{J}_z$ are Hermitian and $[J_x, J_y] = i\hbar J_z$, etc
- The J_is all commute with $\underline{J}^2 = \underline{J}\cdot\underline{J} = J_x^2 + J_y^2 + J_z^2$
- $J_n = \hat{n}\cdot\underline{J}$ where $\hat{n}$ is a unit vector in a given direction
- $[J_n, J_n] \neq 0$ is $\hat{n} \neq \hat{n}$, $[J_n, \underline{J}^2] = 0 \forall\hat{n}$

Consider the Hilbert space $\mathcal{H}$ spanned by the eigenvector of $\underline{J}^2$. Since $\underline{J}^2$ and J_n commute, one can always construct a basis of $\mathcal{H}$ with simultaneous eigenvectors of these two operators. However, since $[J_n, J_m] \neq 0$ if $\hat{n} \neq \hat{m}$, there is no basis of simultaneous eigenvectors of $\underline{J}^2, J_n, J_m$. The simultaneous eigenvectors of $\underline{J}^2$ and J_z are $|jm\rangle$

Consider the ladder operators $J_+ = J_x + iJ_y,\ J_- = J_x - iJ_y,\ J_+ = I_-^\dagger,\ [J_\pm, \underline{J}^2] = 0$ but $[J_+, J_-] \neq 0$. We find through algebraic methods,

1. $$\begin{aligned} J_+|j,m\rangle &\propto \hbar|j,m+1\rangle,\ J_+|jj\rangle = 0 \\ J_-|j,m\rangle &\propto \hbar|j,m-1\rangle,\ J_-|j-j\rangle = 0 \end{aligned}$$
2. The eigenvalues for $\underline{J}^2$ are $j(j+1)\hbar^2$ with $j = 0, \frac{1}{2}, 1, \frac{3}{2}, \cdots$
3. The eigenvectors of J_z are $m\hbar$ with $m = 0, \pm\frac{1}{2}, \pm 1, \pm\frac{3}{2}, \cdots$
4. For simultaneous eigenvector $|jm\rangle$ of $\underline{J}^2$ and J_z, the values of m and j are restricted by the requirement that m in the range $-j \leq m \leq j$

- The eigenvectors $|jm\rangle$ are orthonormal, $\langle j'm'|jm\rangle = \delta_{jj'}\delta_{mm'}$
- $\langle jm|jm\rangle$ has been chosen to equal 1 by choice of normalisation
- For orbital angular momentum, $\underline{L}$:
  - The joint eigenfunctions of $\underline{L}^2$ and L_z are $Y_{lm}(\theta,\phi)$
  - $L_z f(\phi) = -i\hbar\partial_\phi(f(\phi)) = m\hbar f(\phi) \to f(\phi) \propto e^{im\phi}$

- ➥ Because ϕ is a position angle, $e^{im(\phi+2\pi)} = e^{im\phi}$ therefore m must be an integer
- ➥ $\underline{L}^2 Y_{lm} = \hbar^2 l(l+1) Y_{lm}$ and $L_z Y_{lm} = \hbar m Y_{lm}$ for $-l \leq m \leq l$

Lecture 17

Consider $[J_n, \underline{J}^2] = 0$. J_n transforms any eigenvector of $\underline{J}^2$ into an eigenvector of $\underline{J}^2$ belonging to the same value of j, i.e. J^2 is invariant under J_n. Similarly consider a rotation about an axis $\hat{n}$ by an angle θi:

- ➤ $|jm\rangle \to \hat{R}_n(\theta)|jm\rangle$
- ➤ For an infinitesimal transformation - $\hat{R}_n(\epsilon) = \hat{I} - i\epsilon\frac{\hat{J}_n}{\hbar}$
- ➤ For a finite rotation - $\hat{R}_n(\theta) = \exp[-i\theta\hat{J}_n/\hbar]$ * Under a rotation, an eigenstate $|jm\rangle$ transforms into a superposition of $|j'm'\rangle$ with $j = j'$ * $\langle j'm'|J_n|jm\rangle = 0$ when $j \neq j'$

What is the matrix representation of an angular momentum operator?

The $\{|jm\rangle\}$ vectors form an orthonormal basis. For a given value of j, J_n is represented by a $(2j+1)\times(2j+1)$ matrix, since for a given j, m can take $2j+1$ different values and J_n does not couple states of different values of j.

E.g. for $j = \frac{1}{2}$, all the angular momentum operators are represented by a 2×2 matrix. Usually, the basis is chosen to be $\left\{|-\frac{1}{2},\frac{1}{2}\rangle, |\frac{1}{2},-\frac{1}{2}\rangle\right\}$ which can be represented by $|+\rangle, |-\rangle$

- ➤ $J_z|+\rangle = \frac{\hbar}{2}|+\rangle$ where $m = +\frac{1}{2}$ and its state is spin up * $J_z|-\rangle = -\frac{\hbar}{2}|-\rangle$ where $m = -\frac{1}{2}$ and its state is spin down

In this basis, J_z is represented by the matrix:

$$\frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

Similarly,

$$J_x \to \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix};\ J_y \to \frac{\hbar}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}$$

These can be represented using the Pauli Matrices, i.e. $\sigma_x, \sigma_y, \sigma_z$, so $J_i = \frac{\hbar}{2}\sigma_i$

- ➤ $|+\rangle$ is represented by

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

- ➤ and $|-\rangle$ is represented by

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

- ➤ so an arbitrary spin state can be expressed as

$$\alpha|+\rangle + \beta|-\rangle = \begin{pmatrix}\alpha\\ \beta\end{pmatrix}$$

17.1 2 Electron System

Consider 2 electrons $|+\rangle_1$ and $|-\rangle_2$. The system is expressed as $\alpha|+\rangle_1|+\rangle + \beta|+\rangle_1|-\rangle_2 + \gamma|-\rangle_1|+\rangle_2 + \delta|-\rangle_1|-\rangle_2 = |\psi\rangle_{12}$, where $\alpha, \beta, \gamma, \delta$ are complex numbers. More generally, the joint angular momentum state of two particles 1 and is:

$$|\psi\rangle_{12} = \sum_{j_1,m_1,j_2,m_2} c_{j_1 m_1 j_2 m_2}|j_1 m_1\rangle_1 |j_2 m_2\rangle_2$$

$$\underline{J}_1 = (J_{1x}, J_{1y}, J_{1z}) \text{ acts only on } |j_1 m_1\rangle_1$$

$$\underline{J}_2 = (J_{2x}, J_{2y}, J_{2z}) \text{ acts only on } |j_2 m_2\rangle_2$$