3.1 Linear Algebra

Vector spaces

Instead of visualizing a complete set of orthonormal basis functions, $f_\alpha(r)$, consider a set of basis vectors which 'spans a space', $\{|\alpha\rangle\} \longrightarrow$ *e.g.*, $|x\rangle, |y\rangle, |z\rangle$

plus a set of scalars, $\{a\}$, which can be multipliers

basis $\Rightarrow$ a set of 'linearly independent' vectors which spans said space

span $\Rightarrow$ every vector (in this space) can be written as a linear combination of said vectors

vector addition is commutative and associative

scalar multiplication is distributive and associative

within basis $\{|e_i\rangle\}$, an arbitrary vector, $|\alpha\rangle$, can be expressed as $a_i\,|e_i\rangle$, sum implied

Inner products

'inner product' operation: $\langle \alpha \,|\, \beta \rangle$

'norm': $\| \, \alpha \, \| \equiv \sqrt{\langle \alpha \,|\, \alpha \rangle}$, a scalar

norm = 1 $\Rightarrow$ 'normalized'

$\langle \alpha_i \,|\, \alpha_j \rangle \propto \delta_{ij} \Rightarrow$ 'orthogonal'

both properties $\Rightarrow$ 'orthonormal set'

Schwarz inequality: $| \, \langle \alpha \,|\, \beta \rangle \, |^2 \leq \langle \alpha \,|\, \alpha \rangle \langle \beta \,|\, \beta \rangle$

'Linear' transformations

e.g., in three-space,
(a) rotate every vector by A° about $|z\rangle$, or
(b) reflect every vector in xy plane

each vector becomes a new vector (which *could* be identical)

operation: $|e_i'\rangle = \hat{T}\,|e_i\rangle = |e_j\rangle T_{ji}$, sum implied

matrix element $T_{ij} = \{\mathbf{T}\}_{ij} \equiv \langle e_i|\hat{T}|e_j\rangle$

operator $\hat{T} \equiv |e_i\rangle T_{ij}\langle e_j| \Leftrightarrow$ matrix $\mathbf{T}$

matrix addition

matrix multiplication: $\mathbf{U} = \mathbf{ST} \Leftrightarrow U_{ik} = S_{ij}T_{jk}$, sum implied

define components of $|\alpha\rangle$ as a column matrix

transformation rule can be written as $\mathbf{a}' = \mathbf{Ta}$

transpose: $\{\tilde{\mathbf{T}}\}_{ij} \equiv \{\mathbf{T}\}_{ji}$

transpose of a column vector is a row vector

symmetric: $\tilde{\mathbf{T}} = \mathbf{T}$

antisymmetric: $\tilde{\mathbf{T}} = -\mathbf{T}$

conjugate: $\{\mathbf{T}^*\}_{ij} \equiv \{\mathbf{T}\}^*_{ij}$

real: $\mathbf{T}^* = \mathbf{T}$

imaginary: $\mathbf{T}^* = -\mathbf{T}$

Hermitian conjugate (or adjoint): $\{\mathbf{T}^\dagger\}_{ij} \equiv \{\mathbf{T}\}^*_{ji}$

a *square* matrix is Hermitian (or self-adjoint) iff it is equal to its Hermitian conjugate, *i.e.*, $\mathbf{T}^\dagger = \mathbf{T}$

skew-Hermitian: $\mathbf{T}^\dagger = -\mathbf{T}$

in matrix form, $\langle\alpha\,|\,\beta\rangle = \mathbf{a}^\dagger\mathbf{b}$

in general, matrix multiplication is *not* commutative; the difference is called the commutator: $[\mathbf{S},\mathbf{T}] \equiv \mathbf{ST} - \mathbf{TS}$

$(\widetilde{\mathbf{ST}}) = \tilde{\mathbf{T}}\tilde{\mathbf{S}}$

$(\mathbf{ST})^\dagger = \mathbf{T}^\dagger\mathbf{S}^\dagger$

unit matrix is $\mathbf{1}$, where $\{\mathbf{1}\}_{ij} = \delta_{ij}$

inverse, $\mathbf{T}^{-1}$: $\mathbf{T}^{-1}\mathbf{T} = \mathbf{T}\mathbf{T}^{-1} \equiv \mathbf{1}$

inverse exists iff determinant $\neq 0$

$\mathbf{T}^{-1} = (\text{det}\mathbf{T})^{-1}\tilde{\mathbf{C}}$, where $\mathbf{C}$ is matrix of cofactors (see text)

$(\mathbf{ST})^{-1} = \mathbf{T}^{-1}\mathbf{S}^{-1}$

matrix $\mathbf{U}$ is unitary iff $\mathbf{U}^{-1} = \mathbf{U}^\dagger$

consider basis, $\{e_i\}$, and a new basis spanning the same space, $\{f_i\}$:

these bases must be related by a linear transformation, $\mathbf{S} \ni | e_j\rangle = | f_i\rangle S_{ij}$

suppose we have vector $|\alpha\rangle$, expressed using basis $\{e_i\}$: $|\alpha\rangle = a_i^e \,|e_i\rangle$

then $|\alpha\rangle = a_i^e \,| f_j\rangle S_{ji}$, or $a_j^f = S_{ji} a_i^e$, or $\mathbf{a}^f = \mathbf{S}\mathbf{a}^e$

remember $\hat{T}$: in old basis, $\mathbf{a}'^e = \mathbf{T}^e \mathbf{a}^e$

in new basis, $\mathbf{a}'^f = \mathbf{S}\mathbf{a}'^e = \mathbf{S}(\mathbf{T}^e\mathbf{a}^e) = \mathbf{S}\mathbf{T}^e\mathbf{S}^{-1}\mathbf{a}^f$

$\therefore \mathbf{T}^f = \mathbf{S}\mathbf{T}^e\mathbf{S}^{-1}$; or $\mathbf{T}^f$ and $\mathbf{T}^e$ are ‘similar’

also, both bases are orthonormal iff $\mathbf{S}$ is unitary

furthermore, det($\mathbf{T}^f$)=det($\mathbf{T}^e$) and Tr($\mathbf{T}^f$)=Tr($\mathbf{T}^e$)

Eigenvectors and Eigenvalues

Consider a particular linear transformation, a rotation by θ about some axis in three-space:

all vectors will travel around a cone about the axis of rotation–except those vectors *on* that axis, which are unchanged

those special vectors which transform into simple multiples of themselves, $\hat{T}\,|\alpha\rangle = \lambda\,|\alpha\rangle$, are called *eigenvectors* of the transformation, while the (complex) λ are called *eigenvalues*

With respect to a *particular* basis, the eigenstates of $\hat{T}$ can be found from $\mathbf{Ta} = \lambda\mathbf{a}$, or $(\mathbf{T} - \lambda\mathbf{1})\mathbf{a} = \mathbf{0}$:

if $\mathbf{a} \neq \mathbf{0}$, then $(\mathbf{T} - \lambda\mathbf{1})^{-1}$ must be singular and $\det(\mathbf{T} - \lambda\mathbf{1}) = \mathbf{0}$

this last condition leads to all the eigenvalues and eigenvectors of $\hat{T}$ *in that basis*

If $\mathbf{T}$ is diagonalizable, then there is a similarity matrix which transforms it into diagonal form $= \mathbf{STS}^{-1}$

Hermitian Transformations

Consider the basis $\{i\}$, which spans the space of interest:
$\langle\alpha|\,\hat{T}\,|\beta\rangle = \langle\alpha|i\rangle\langle i|\,\hat{T}\,|j\rangle\langle j|\,\beta\rangle = \alpha_i{}^* T_{ij}\beta_j =$
$(\alpha_i T_{ij}{}^*)^*\beta_j = (\alpha_i\{\mathbf{T}^\dagger\}_{ji})^*\beta_j = (\{\mathbf{T}^\dagger\}_{ji}\alpha_i)^*\beta_j$

i.e., $\hat{T}^\dagger$ is that transformation which, when applied to the first member of an inner product, gives the same result as if $\hat{T}$ itself had been applied to the second vector.

Four properties:

1. any Hermitian matrix can be diagonalized by a similarity transformation;
2. the eigenvalues of a Hermitian transformation are real;
3. the eigenvectors of a Hermitian transformation belonging to distinct eigenvalues are orthogonal; the other eigenvectors can be made orthogonal using procedure of Gram-Schmidt;
4. the eigenvectors of a Hermitian transformation span the space.
   NB, #4 is true only for finite-dimensional spaces

3.2 Function Spaces

It is possible to define certain classes of functions so that they constitute a vector space:

e.g., all polynomials on $x = (-1, 1)$ of degree $< N$, $P(N)$, or
all odd functions that $= 0$ at $x = 1$, or
all periodic functions with period π.

It is necessary that they span the space and convenient that they be orthonormal.

Linear operators (such as $\hat{x}$ or $\hat{D} \equiv d/dx$) behave as linear transformations if they carry functions in this space into other members of the space.

Note that the operator $\hat{x}$ is *not* linear *in* $P(N)$ since it is able to promote the $(N-1)^{\text{th}}$-order polynomial into the N^{th}-order polynomial, which is *not* a member of $P(N)$.

But, $\hat{x}$ *is* linear in $P(\infty)$

$\hat{x}$ is also Hermitian in $P(\infty)$

Note, however, that it has *no* eigenfunctions in $P(\infty)$!

In fact, it can be shown that the eigenfunctions of $\hat{x}$ are Dirac delta functions

In general, in infinite-dimensional spaces some Hermitian operators have complete sets of eigenvectors, some have incomplete sets, and others have no eigenvectors at all (in that space).

Unfortunately, the completeness property is *essential* in quantum mechanical applications. This will be discussed more shortly.

Hilbert spaces

A *complete inner product space* is called a Hilbert space.

$P(\infty)$ can be *completed* by adding the remainder of the square-integrable functions on the interval $x = (-1, 1)$: $L_2(-1, 1)$.

We are concerned with the particular Hilbert space, $L_2(-\infty, \infty)$.

The eigenfunctions of the Hermitian operators $i\widehat{D} = id/dx$ and $\widehat{x} = x$ are $f_\lambda(x) = A_\lambda e^{-i\lambda x}$ and $g_\lambda(x) = B_\lambda \delta(x - \lambda)$, respectively.

Every real number is an eigenvalue of $i\widehat{D}$, and every real number is an eigenvalue of $\widehat{x}$. The set of eigenvalues of an operator is called its spectrum; $i\widehat{D}$ and $\widehat{x}$ are operators with continuous spectra.

Unfortunately, these eigenfunctions are not square integrable on $x = (-1, 1)$, and therefore they *do not lie in Hilbert space*.

It is customary to 'orthonormalize' these (fundamentally unnormalizable) functions to the Dirac delta function:
$\langle f_\lambda | f_\mu \rangle = \delta(\lambda - \mu), A_\lambda = (2\pi)^{-1/2}$ and
$\langle g_\lambda | g_\mu \rangle = \delta(\lambda - \mu), B_\lambda = 1$

Importantly, these two *complete* sets of 'nearly orthonormalized' functions are *useful* in quantum mechanics.

Their continuous eigenvalue spectra necessitate changing the sum over discrete eigenstates into an integral over continuous eigenstates:

$$\hat{1} = \int_{-\infty}^{\infty} d\lambda \ |f_\lambda\rangle\langle f_\lambda| = \int_{-\infty}^{\infty} d\lambda \ |g_\lambda\rangle\langle g_\lambda|$$

3.3 Statistical Interpretation

Postulates:

1. The state of a particle is represented by a normalized vector, $|\Psi\rangle$, in the Hilbert space L_2.

2. Observables $Q(x,p,t)$ are represented by $\widehat{Q}(x,(\hbar/i)(\partial/\partial x),t)$; the expectation value of Q in the state Ψ is

$$\langle Q\rangle_\Psi = \int dx\, \Psi(x,t)^* \widehat{Q} \Psi(x,t) = \langle \Psi |\, \widehat{Q}\, | \Psi\rangle$$

3. If you measure Q for particle in state Ψ, you *must* get one of the eigenvalues of $\widehat{Q}$. The probability of getting a particular eigenvalue λ is equal to absolute square of the λ component of Ψ when expressed in orthonormal basis of eigenvectors.

Clearly, the eigenfunctions of any operator representing an observable *must* form a complete set.

$\widehat{Q}\,|e_n\rangle = \lambda_n\,|e_n\rangle$, $\langle e_n|e_m\rangle = \delta_{nm}$, and $|\Psi\rangle = c_n\,|e_n\rangle$ imply that the probability of getting one particular eigenvalue λ_n $=|c_n|^2=|\langle e_n \mid \Psi\rangle|^2$

3.4 Uncertainty Principle

For any two observables, $\sigma_A^2 \sigma_B^2 \geq (\langle[\hat{A}, \hat{B}]\rangle / 2i)^2$.

Observables such that their operators do not commute are called *incompatible*; it is not possible to find a complete basis set in which both operators are diagonal.

Conversely, observables such that their operators commute *can* be diagonalized simultaneously, leading to a complete set of common eigenfunctions.

Moreover, in those cases where the operators do not commute, it is possible to define a minimum uncertainty wavepacket.

The energy-time uncertainty principle relates the time it takes *any* observable of a system to change appreciably, $\Delta t = \frac{\sigma_Q}{|d\langle Q\rangle/dt|}$, to the corresponding uncertainty in a measurement of that system's energy: $\Delta E \, \Delta t \geq \hbar/2$.

NB, this principle *does not* imply that energy conservation can be "suspended" to the extent of ΔE for a time Δt.