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’, \( \{|\alpha\rangle\} \rightarrow \text{e.g.}, |x\rangle, |y\rangle, |z\rangle \)

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 \( A^\circ \) about \( |z\rangle \), or
(b) reflect every vector in \( xy \) plane

each vector becomes a new vector (which \textit{could} be identical)

operation: \( |e'_i\rangle = \hat{T} |e_i\rangle = |e_j\rangle T_{ji} \), sum implied

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

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

matrix addition

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

define components of \( |\alpha\rangle \) as a column matrix

transformation rule can be written as \( a' = Ta \)
transpose: \( \{\tilde{T}\}_{ij} \equiv \{T\}_{ji} \)

transpose of a column vector is a row vector

symmetric: \( \tilde{T} = T \)

antisymmetric: \( \tilde{T} = -T \)

conjugate: \( \{T^*\}_{ij} \equiv \{T\}_{ij}^* \)

real: \( T^* = T \)

imaginary: \( T^* = -T \)

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

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

skew-Hermitian: \( T^\dagger = -T \)

in matrix form, \( \langle \alpha \vert \beta \rangle = a^\dagger b \)
in general, matrix multiplication is *not* commutative; the difference is called the commutator: \([S, T] \equiv ST - TS\)

\((ST) = \tilde{T}\tilde{S}\)

\((ST)^\dagger = T^\dagger S^\dagger\)

unit matrix is 1, where \(\{1\}_{ij} = \delta_{ij}\)

inverse, \(T^{-1}: T^{-1}T = TT^{-1} \equiv 1\)

inverse exists iff determinant \(\neq 0\)

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

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

matrix \(U\) is unitary iff \(U^{-1} = U^\dagger\)
consider basis, \( \{ e_i \} \), and a new basis spanning the same space, \( \{ f_i \} \):

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

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 \( a_j^f = S a_i^e \)

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

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

\( \therefore T^f = ST^e S^{-1} \); or \( T^f \) and \( T^e \) are ‘similar’

also, both bases are orthonormal iff \( S \) is unitary

furthermore, \( \det(T^f) = \det(T^e) \) and \( \text{Tr}(T^f) = \text{Tr}(T^e) \)
Eigenvectors and Eigenvalues

Consider a particular linear transformation, a rotation by $\theta$ 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) $\lambda$ are called eigenvalues

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

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

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

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

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

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 $\pi$.

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 $(N - 1)^{th}$-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 \( i \hat{D} = id/dx \) and \( \hat{x} = x \) 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 \( i \hat{D} \), and every real number is an eigenvalue of \( \hat{x} \). The set of eigenvalues of an operator is called its spectrum; \( i \hat{D} \) and \( \hat{x} \) 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:

$$\langle f_\lambda | f_\mu \rangle = \delta(\lambda - \mu), A_\lambda = (2\pi)^{-1/2} \text{ and } \langle g_\lambda | g_\mu \rangle = \delta(\lambda - \mu), B_\lambda = 1$$

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 $\hat{Q}(x, (\hbar/i)(\partial/\partial x), t)$; the expectation value of $Q$ in the state $\Psi$ is

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

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

Clearly, the eigenfunctions of any operator representing an observable must form a complete set.
\[ \hat{Q} |e_n\rangle = \lambda_n |e_n\rangle, \quad \langle e_n | e_m \rangle = \delta_{nm}, \text{ and} \]
\[ |\Psi\rangle = c_n |e_n\rangle \text{ imply that the probability of getting one particular eigenvalue } \lambda_n \]
\[ = |c_n|^2 = |\langle e_n | \Psi \rangle|^2 \]
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 $\Delta E$ for a time $\Delta t$. 