Infinite-Dimensional Vector Spaces

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In QM, we will often need to solve first-order linear differential equations of the following kind:

\[ i \frac{d}{dt} |\psi(t)\rangle = \Omega |\psi(t)\rangle, \]

where operator \( \Omega \) is *time-independent* and *Hermitian*.

The formal solution of this equation is

\[ |\psi(t)\rangle = e^{-i\Omega t} |\psi_0\rangle, \]

where vector \(|\psi_0\rangle = |\psi(0)\rangle\) represents the initial conditions.

Using the completeness relation for the eigenbasis of \( \Omega \),

\[ |\psi(t)\rangle = e^{-i\Omega t} \left( \sum_i |\omega_i\rangle \langle \omega_i| \right) |\psi_0\rangle \]
Note that $\Omega^n |\omega_i\rangle = \omega_i^n |\omega_i\rangle$, so that $f(\Omega)|\omega_i\rangle = f(\omega_i)|\omega_i\rangle$. Therefore, $e^{-i\Omega t}|\omega_i\rangle = e^{-i\omega_i t}|\omega_i\rangle$. In this manner, the solution of the differential equation can be written as

$$|\psi(t)\rangle = \sum_i e^{-i\omega_i t} |\omega_i\rangle \langle \omega_i | \psi_0 \rangle = \sum_i \beta_i e^{-i\omega_i t} |\omega_i\rangle$$

where $\beta_i = \langle \omega_i | \psi_0 \rangle$ are the expansion coefficients of $|\psi_0\rangle$ in the $|\omega_i\rangle$ basis.

Operator $U(t) = e^{-i\Omega t} = \sum_i e^{-i\omega_i t} |\omega_i\rangle \langle \omega_i |$ is called the propagator:

$$|\psi(t)\rangle = U(t)|\psi_0\rangle$$

In classical dynamics, eigenvalues $\omega_i$ are known as the frequencies of free vibrations and corresponding eigenvectors $|\omega_i\rangle$ are known as the normal modes.
Discretized String Displacements

A clamped string:

- We can consider the space of functions for which \( f(0) = f(L) = 0 \).

- Basis vectors: \( |x_i\rangle \rightarrow \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix} \)

- Note that the basis vectors are labeled by location, but the vector space is defined for function values, not for locations:

\[
|f\rangle = \sum_i f(x_i) |x_i\rangle
\]

- Properties of the basis vectors:

\[
\langle x_i | x_j \rangle = \delta_{ij} \quad \text{(normalization)}
\]

\[
\sum_i |x_i\rangle \langle x_i| = I \quad \text{(completeness)}
\]
Discretized String Displacements (Cont’d)

- Using this basis,

\[ \langle x_j | f \rangle = \sum_i f(x_i) \langle x_j | x_i \rangle = \sum_i f(x_i) \delta_{ji} = f(x_j) \]

- Inner product:

\[ \langle g | f \rangle = \langle g \left( \sum_i |x_i\rangle \langle x_i | \right) f \rangle = \sum_i g^*(x_i) f(x_i) \]

- We want to take the number of discretization intervals to \( \infty \), but then we encounter a problem: \( \langle g | f \rangle \rightarrow \infty \) as well.
The “obvious” fix to the inner product problem is to redefine the inner product via

$$\langle g | f \rangle = \int_0^L g^*(x)f(x)dx.$$ 

Note, however, that this fix involves some serious assumptions:

- Uniformity of space
- Infinite divisibility of space

If we do this, how do we express the normalization and completeness of the basis?
Continuous String Displacements (Cont’d)

- The appropriate completeness relation is

$$\int_0^L |x\rangle\langle x| dx = I$$

Indeed,

$$\langle g | f \rangle = \langle g \left( \int_0^L |x\rangle\langle x| dx \right) f \rangle = \int_0^L g^*(x)f(x)dx$$

- To fix the normalization, consider

$$f(x) = \langle x | f \rangle = \langle x \left( \int_0^L |x'|\langle x'|dx' \right) f \rangle = \int_0^L \langle x|x'\rangle f(x')dx'$$

To make this work, we need to postulate

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

where $\delta(x - x')$ is the Dirac delta function. It can be convenient to think that $\delta(x - x')$ is a function of $x'$ with parameter $x$. 
Some Properties of the Dirac Delta Function

I often find it convenient to think that 
\[ \delta(x) = \lim_{\Delta \to 0} f_\Delta(x), \]
where \( f_\Delta(x) \) is the unit area triangle function. See figure on the left.

\( \delta(x) \) is even. \( \delta(x - x') = \delta(x' - x) \).

According to the rules of differentiation under the integral,
\[ \int \left( \frac{d}{dx} \delta(x - x') \right) f(x') dx' = \frac{d}{dx} \int \delta(x - x') f(x') dx' = \frac{df(x)}{dx}. \]
Following Shankar, we will utilize the notation
\( \delta'(x - x') \equiv \frac{d}{dx} \delta(x - x') \), i.e., the differentiation is performed w.r.t. the first argument.

\( \delta'(x) \) is odd. \( \delta'(x - x') = -\delta'(x' - x) \).

\( \delta'(x - x') = \delta(x - x') \frac{d}{dx}. \) This can be extended to derivatives of arbitrary order:
\[ \delta^{(n)}(x - x') = \delta(x - x') \frac{d^n}{dx'^n}. \]
Some Properties of the Dirac Delta Function (Cont’d)

\[ \delta(ax) = \frac{\delta(x)}{|a|} \quad (a \text{ is a real constant}) \]

\[ \delta(f(x)) = \sum_{f(x_i)=0} \frac{\delta(x_i)}{|f'(x_i)|} \]

\[ \delta(x - x') = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-x')} \, dk \]

The last formula can be derived from the definition of the continuous Fourier transform:

\[ f(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx'} f(x') \, dx' \]

\[ f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} f(k) \, dk = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{ikx} e^{-ikx'} f(x') \, dx' \, dk \]

Therefore, we must have \[ \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} e^{-ikx'} \, dk = \delta(x - x') \].
Dirac Delta Function in a Countable Basis

- Suppose, there exists a complete, countable orthonormal basis $|\varphi_n\rangle$ such that $\langle \varphi_m | \varphi_n \rangle = \delta_{mn}$. For example, for the displacements of the clamped string, $\varphi_n \to \sqrt{\frac{2}{L}} \sin \left( \frac{\pi nx}{L} \right)$. If the string ends are not clamped, $\varphi_n$ are the orthonormal shifted Legendre polynomials.
- For some arbitrary vector $|f\rangle$,

\[
\langle x | f \rangle = \langle x \sum_{n} |\varphi_n\rangle \langle \varphi_n | f \rangle = \int \sum_{n} \langle x | \varphi_n \rangle \langle \varphi_n | x' \rangle \langle x' | f \rangle dx'
\]

\[
f(x) = \int \sum_{n} \varphi_n(x) \varphi_n^*(x') f(x') dx'
\]

Therefore, for any such basis,

\[
\delta(x - x') = \sum_{n} \varphi_n(x) \varphi_n^*(x')
\]
Operators in Infinite-Dimensional Vector Spaces

- For QM, we will need the differential operator:

\[
\left\langle \frac{df}{dx} \right\rangle = D|f\rangle
\]

- How does \( D \) look like for the discretized string?

- For the continuous string, we want

\[
\frac{df(x)}{dx} = \langle x|D|f\rangle
\]

\[
\frac{df(x)}{dx} = \langle x|D \left( \int_0^L |x'|\langle x'|dx' \right) f\rangle
\]

\[
\frac{df(x)}{dx} = \int_0^L \langle x|D|x'\rangle \langle x'|f\rangle dx' = \int_0^L \langle x|D|x'\rangle f(x') dx'
\]

Therefore, in the \(|x\rangle\) basis

\[
D_{xx'} \equiv \langle x|D|x'\rangle = \delta'(x - x') = \delta(x - x') \frac{d}{dx'}
\] (1)
Hermitian Differential Operator

- $D$ is (mostly) anti-Hermitian, as $D_{x'x}^* = \delta^*(x' - x) = -\delta'(x - x') = -D_{xx'}$.

- We can hope that operator $K = -iD$ is Hermitian. However, from the discretized representation one can already expect that there could be problems at the edges.

- In order to have $K = K^\dagger$, we should require
  \[
  \langle g | K | f \rangle = \langle Kf | g \rangle^* = \langle f | K^\dagger | g \rangle^* = \langle f | K | g \rangle^*
  \]
  for arbitrary vectors $|f\rangle$ and $|g\rangle$. Is this really the case? Note that
  \[
  \langle g | K | f \rangle = \int_0^L \int_0^L \langle g | x \rangle \langle x | K | x' \rangle \langle x' | f \rangle \, dx \, dx' = \int_0^L g^*(x) \left(-i \frac{df(x)}{dx}\right) \, dx
  \]
  Integrating by parts,
  \[
  \langle g | K | f \rangle = -ig^*(x)f(x) \bigg|_0^L + \int_0^L \frac{dg^*(x)}{dx} f(x) \, dx \quad (2)
  \]
  On the other hand,
  \[
  \langle f | K | g \rangle^* = \left( \int_0^L f^*(x) \left(-i \frac{dg(x)}{dx}\right) \, dx \right)^* = i \int_0^L \frac{dg^*(x)}{dx} f(x) \, dx \quad (3)
  \]
Comparing Eqs. 2 and 3, we can conclude that operator $K$ is Hermitian only if the *surface term* $-ig^*(x)f(x)|_0^L$ vanishes: $g^*(L)f(L) = g^*(0)f(0)$.

The Hermiticity requirement imposed on $K$ restricts the space of possible functions. What kind of functions supported on $[0, L]$ can we use? What if the functions are defined on a circle and $K = -i \frac{d}{d\phi}$?

For functions defined on $[-\infty, \infty]$, the surface term obviously vanishes if $\lim_{|x| \to \infty} f(x) = 0$. But we will also be interested in the functions that behave at infinity as $e^{ikx}$, with real parameter $k$. We will assume that in QM applications $K$ remains Hermitian for such functions. Note that, if $f(x) \propto e^{ikx}$ and $g(x) \propto e^{ik'x}$ then $g^*(x)f(x) \propto e^{i(k-k')x}$, and the surface term oscillates. If necessary, however, we can perform various calculations by replacing $k - k'$ with $k - k' + i \varepsilon \text{sign}(x)$ and then take the limit $\varepsilon \to 0$ in the final answer.
Eigenvalues and Eigenvectors of $K$

- Eigenvalues and eigenvectors of $K$ are defined by
  \[ K |k\rangle = k |k\rangle \]

- In the $|x\rangle$ basis we have
  \[ \langle x | K | k \rangle = k \langle x | k \rangle \]
  \[ \int \langle x | K | x' \rangle \langle x' | k \rangle dx' = k \psi_k(x) \]
  \[ -i \frac{d}{dx} \psi_k(x) = k \psi_k(x) \]
  \[ \psi_k(x) = Ae^{ikx} \quad (A \text{ is a scalar constant}) \]

- We will restrict possible values of $k$ to real numbers using the requirement that operator $K$ must remain Hermitian in the space of $\psi_k(x)$ functions. This requirement defines the physical Hilbert space, which is of interest in QM.
We will choose \( A = \frac{1}{\sqrt{2\pi}} \) in order to have \( \langle k|k' \rangle = \delta(k - k') \). Indeed,

\[
\langle k|k' \rangle = \int \langle k|x \rangle \langle x|k' \rangle dx = \int \psi_k^*(x)\psi_{k'}(x) dx
\]

\[
= \frac{1}{2\pi} \int e^{i(k' - k)x} dx = \delta(k - k')
\]

Operator \( K \) generates a basis \( |k\rangle \) normalized by \( \langle k|k' \rangle = \delta(k - k') \), the closest thing to orthonormal for a continuous spectrum of eigenvalues. In this basis,

\[
f(k) = \langle k|f \rangle = \int_{-\infty}^{\infty} \langle k|x \rangle \langle x|f \rangle dx = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} f(x) dx.
\]

Thus \( f(k) \) is just the Fourier transform of \( f(x) \).

Matrix elements of \( K \) in the \( |k\rangle \) basis:

\[
K_{kk'} = \langle k|K|k' \rangle = k' \langle k|k' \rangle = k' \delta(k - k')
\]
Operator $X$

- We can also introduce operator $X$ with eigenvalues and eigenvectors formally satisfying the equation

$$X|x\rangle = x|x\rangle$$

and with matrix elements

$$X_{xx'} = \langle x|X|x'\rangle = x'\langle x|x'\rangle = x'\delta(x - x')$$

- The action of operator $X$ on $|f\rangle$ can be seen in the $|x\rangle$ basis:

$$\langle x|X|f\rangle = \int \langle x|X|x'\rangle \langle x'|f\rangle dx' = \int x'\delta(x - x')f(x')dx' = xf(x)$$

- For completeness, it is good to note that

$$K_{xx'} = \langle x|K|x'\rangle = -i\delta'(x - x') \quad \text{(this follows from Eq. 1)}$$

$$X_{kk'} = \langle k|X|k'\rangle = \int \langle k|x\rangle \langle x|X|k'\rangle dx = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ikx} x e^{ik'x} dx$$

$$= i \frac{d}{dk} \left[ \frac{1}{2\pi} \left( \int_{-\infty}^{\infty} e^{i(k'-k)x} dx \right) \right] = i\delta'(k - k')$$
Commutator $[X, K]$

In the $|x\rangle$ basis,

$$X|f\rangle \rightarrow xf(x)$$

$$K|f\rangle \rightarrow -i \frac{d}{dx} f(x)$$

$$XK|f\rangle \rightarrow -ix \frac{d}{dx} f(x)$$

$$KX|f\rangle \rightarrow -i \frac{d}{dx} (xf(x)) = -ix \frac{d}{dx} f(x) - if(x)$$

$$[X, K]|f\rangle = (XK - KX)|f\rangle \rightarrow if(x)$$

As $|f\rangle$ is an arbitrary vector and $i$ is a basis-independent scalar, we must have (assuming completeness of the $|x\rangle$ basis)

$$[X, K] = il$$

Note that $\text{tr}([X, K]) = i\infty$ while in a finite-dimensional space $\text{tr}([\Omega, \Lambda]) = 0$ for arbitrary $\Omega$ and $\Lambda$. 
Determines $[X, K^2]$. 

Determine $[g(X), K]$. 

Determine eigenvalues and eigenvectors for the operator $\Lambda = \alpha K + \beta X$, where $\alpha$ and $\beta$ are real numbers.
Operator of Translations

- Operator of translations is defined by its representation in the $|x\rangle$ basis: $T_a \rightarrow e^{-a \frac{d}{dx}} = e^{-iaK}$. $T_a$ is unitary.
- Its action on some vector $|f\rangle$ can be understood from the following:

$$\langle x|T_a|f\rangle = f(x) - a \frac{d}{dx} f(x) + \frac{a^2}{2!} \frac{d^2}{dx^2} f(x) - \cdots$$

This is just the Taylor series for $f(x-a)$ about the point $x$, so

$$\langle x|T_a|f\rangle = f(x - a)$$

If, let say, $f(x)$ is centered at 0 then $f(x-a)$ is centered at $a$. Therefore, $T_a$ shifts the vector $|f\rangle$ by $a$.

- As one might expect, $T_a T_b = e^{-iaK} e^{-ibK} = e^{-i(a+b)K} = T_{a+b}$.
- What are the eigenvalues and eigenvectors of $T_a$?
The parity operator $\Pi$ is defined by its action on the $|x\rangle$ basis vectors:

$$\Pi |x\rangle = |-x\rangle$$

To avoid possible confusion, it is important to note that $|-x\rangle \neq -|x\rangle$.

Matrix elements:

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

The action of parity operator on some vector $|f\rangle$ can be understood in the $|x\rangle$ basis:

$$\langle x|\Pi|f\rangle = \int \langle x|\Pi|x'\rangle \langle x'|f\rangle dx' = \int \delta(x + x') f(x') dx' = f(-x)$$

Is parity operator Hermitian? Is it unitary?
Eigenvalues and Eigenvectors of $\Pi$

- Eigenvalues and eigenvectors of $\Pi$ are defined by
  \[
  \Pi |\pi\rangle = \pi |\pi\rangle \\
  \Pi^2 |\pi\rangle = \pi \Pi |\pi\rangle = \pi^2 |\pi\rangle
  \]

  As $\Pi^2 = I$, $\pi^2 = 1$. Therefore, $\pi = \pm 1$.

- To determine the eigenvectors, consider
  \[
  \langle x | \Pi | \pi \rangle = \pi \langle x | \pi \rangle \\
  \int \langle x | \Pi | x' \rangle \langle x' | \pi \rangle dx' = \pi \pi(x) \\
  \int \delta(x + x') \pi(x') dx' = \pi \pi(x) \\
  \pi(-x) = \pi \pi(x)
  \]

  $\pi(-x) = \pi(x)$ if $\pi = 1$ (any even function) \\
  $\pi(-x) = -\pi(x)$ if $\pi = -1$ (any odd function)
Next class (09/08/20) — homework discussion. Please have your homework solutions in a form that can be shared in Zoom.

Exercises, problem solving, etc.