PHY 712 Quantum Mechanics
12-12:50 PM MWF Olin 103

Plan for Lecture 3:
Reading: Chapter 1 in Shankar

1. **Evaluation of operators and functions of operators**
2. **Continuum bases**

PHY 741 Quantum Mechanics

MWF 12 PM - 12:50 PM	OPL 103	http://www.wfu.edu/~natalie/f17phy741/

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Course schedule

(Preliminary schedule -- subject to frequent adjustment.)

	Date	F&W Reading	Topic	Assignment	Due
1	Mon, 8/28/2017	Chap. 1	Review of basic principles	#1	9/6/2017
2	Wed, 8/30/2017	Chap. 1	Linear vector spaces	#2	9/6/2017
3	Fri, 9/01/2017	Chap. 1	Linear vector spaces	#3	9/6/2017
4	Mon, 9/04/2017				
5	Wed, 9/06/2017				
6	Fri, 9/08/2017				

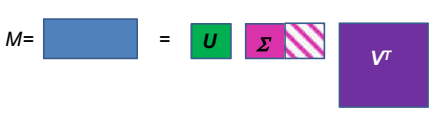
Correction to Wednesday's lecture:
Note that:

$$MM^T = U\Sigma V^T \left(U\Sigma V^T\right)^T = U\Sigma V^T V\Sigma U^T = U\Sigma^2 U^T$$

$$M^T M = \left(U\Sigma V^T\right)^T U\Sigma V^T = V\Sigma U^T U\Sigma V^T = V\Sigma^2 V^T$$

$\Rightarrow$ By convention, singular values are chosen as $\sigma_i \geq 0$

Note that SVD can be applied to rectangular matrices



Further relationships:

$$MM^T = U\Sigma V^T \left(U\Sigma V^T\right)^T = U\Sigma V^T V\Sigma U^T = U\Sigma^2 U^T$$

$$M^T M = \left(U\Sigma V^T\right)^T U\Sigma V^T = V\Sigma U^T U\Sigma V^T = V\Sigma^2 V^T$$

Note that: if M is Hermitian, $M = M^\dagger$

$\Rightarrow$ In this case, $U = V$ and the singular values are equal to the squares of the eigenvalues: $\sigma_i = \lambda_i^2$

"Proof" that Hermitial matrices have real eigenvalues

Suppose we have a Hermitian matrix H such that $H = H^\dagger$

Also suppose we have found an eigenvalue λ and eigenvector $|\psi$

$H|\psi_\lambda\rangle = \lambda|\psi_\lambda\rangle$

Conjugate equation: $\langle\psi_\lambda|H^\dagger = \lambda^*\langle\psi_\lambda|$

$$\langle\psi_\lambda|H|\psi_\lambda\rangle = \lambda\langle\psi_\lambda|\psi_\lambda\rangle$$

$$\langle\psi_\lambda|H^\dagger|\psi_\lambda\rangle = \lambda^*\langle\psi_\lambda|\psi_\lambda\rangle$$

$$\|$$

$$\langle\psi_\lambda|H|\psi_\lambda\rangle = \lambda^*\langle\psi_\lambda|\psi_\lambda\rangle \quad \Rightarrow \lambda = \lambda^*$$

Functions of Operators

An operator $\mathbf{O}$ can generally be evaluated within a spanning orthonormal basis:

$$\mathbf{O} = \sum_{i,j=1}^{n} |i\rangle O_{ij} \langle j| \quad \text{where} \quad O_{ij} \equiv \langle i|\mathbf{O}|j\rangle$$

It is often convenient to choose the spanning orthnormal basis from the eigenvectors:

$$\mathbf{O}|\Psi_\alpha\rangle = \lambda_\alpha|\Psi_\alpha\rangle$$

$$\Rightarrow \mathbf{O} = \sum_{\alpha=1}^{n} \lambda_\alpha |\Psi_\alpha\rangle\langle\Psi_\alpha|$$

How can we evaluate functions of operators?

Assume that $f(\mathbf{O}) = f(0) + \mathbf{O}f'(0) + \frac{1}{2}\mathbf{O}^2 f''(0) + \frac{1}{3!}\mathbf{O}^3 f'''(0) + \cdots$

Properties of eigenvectors:

$$\mathbf{O}|\Psi_\alpha\rangle = \lambda_\alpha |\Psi_\alpha\rangle$$
$$\mathbf{O}^2|\Psi_\alpha\rangle = \lambda_\alpha^2 |\Psi_\alpha\rangle$$
$$\mathbf{O}^3|\Psi_\alpha\rangle = \lambda_\alpha^3 |\Psi_\alpha\rangle \quad \cdots$$

Example:

$$e^{\mathbf{O}} = 1 + \mathbf{O} + \frac{1}{2}\mathbf{O}^2 + \frac{1}{3!}\mathbf{O}^3 + \cdots$$

Functions of multiple operators

If operators commute, $\mathbf{AB} = \mathbf{BA}$, their functions can be combined in the usual. For example, in this case, it can be shown that

$$e^{a\mathbf{A}+b\mathbf{B}} = e^{a\mathbf{A}}e^{b\mathbf{B}}$$

However, if the operators do not commute, $\mathbf{AB} \neq \mathbf{BA}$, combination of functions becomes much more complicated. For example, if $\mathbf{A}$ and $\mathbf{B}$ do not commute, but commute with their commutator $[\mathbf{A},\mathbf{B}] \equiv \mathbf{AB} - \mathbf{BA}$, then:

$$e^{a\mathbf{A}}e^{b\mathbf{B}} = e^{a\mathbf{A}+b\mathbf{B}+(ab/2)[\mathbf{A},\mathbf{B}]}.$$

This is a famous result attributed to Baker, Cambell, and Hausdorff

It is possible to find various clever proofs of this identity in the literature.
For plausibility, we can consider the first few terms of the Taylor exansion:
Taylor expansion of $e^{a\mathbf{A}}e^{b\mathbf{B}} = e^{a\mathbf{A}+b\mathbf{B}+(ab/2)[\mathbf{A},\mathbf{B}]}$

$$e^{a\mathbf{A}}e^{b\mathbf{B}} = \left(1 + a\mathbf{A} + \frac{1}{2}a^2\mathbf{A}^2\cdots\right)\left(1 + b\mathbf{B} + \frac{1}{2}b^2\mathbf{B}^2\cdots\right)$$
$$= 1 + a\mathbf{A} + b\mathbf{B} + ab\mathbf{AB} + \cdots$$

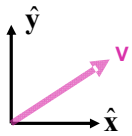
$$e^{a\mathbf{A}+b\mathbf{B}+(ab/2)[\mathbf{A},\mathbf{B}]} = 1 + a\mathbf{A} + b\mathbf{B} + \frac{ab}{2}(\mathbf{AB} - \mathbf{BA}) + \frac{1}{2}\left(a\mathbf{A} + b\mathbf{B} + \frac{ab}{2}(\mathbf{AB} - \mathbf{BA})\right)^2 + \cdots$$

$$\frac{1}{2}\left(a^2\mathbf{A}^2 + b^2\mathbf{B}^2 + ab(\mathbf{AB} + \mathbf{BA}) + \cdots\right)$$

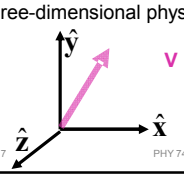
$$= 1 + a\mathbf{A} + b\mathbf{B} + ab\mathbf{AB} + \cdots$$

Examples of finite dimensional vector spaces

Two-dimensional physical space



Three-dimensional physical space



Notion of a set of vectors which may or may not "span" the vector space.

Consider the following three vectors and determine whether the space the 3-dimensional vector space?

$$|v_1\rangle = \hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}}$$
$$|v_2\rangle = \hat{\mathbf{x}} - \hat{\mathbf{y}} - \hat{\mathbf{z}}$$
$$|v_3\rangle = \hat{\mathbf{x}}$$

Notion of "completeness" –
In this example $|v_1\rangle$, $|v_2\rangle$, and $|v_3\rangle$, are not "complete"; they do not span the 3-dimensional vector space.

Examples of finite dimensional vector spaces

Vector spaces constructed with orthonormal functions usually defined in a fixed region of space.

For example, consider the one-dimensional functions defined in the range $0 \le x \le L$:

$$f_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi n x}{L}\right)$$

$$\langle f_n(x) | f_{n'}(x) \rangle = \delta_{nn'}$$

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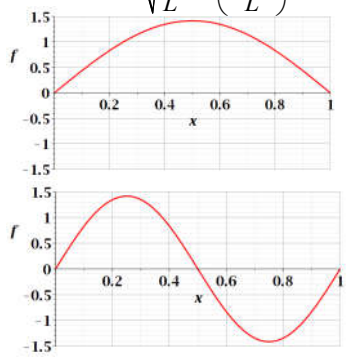
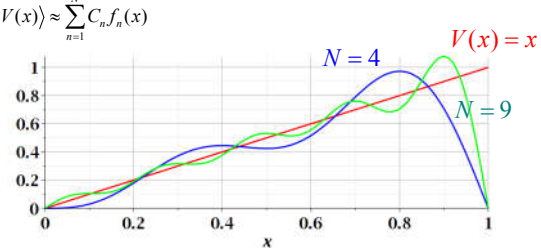


Any one-dimensional function $|V(x)\rangle$ defined within $0 \le x \le L$ can be well represented as a linear combination of these basis functions:

$$|V(x)\rangle \approx \sum_{n=1}^{N} C_n f_n(x)$$



In this case, the vector space becomes "complete" as $N \to \infty$

Relationship between the finite and continuous systems
Kronecker ←→ Dirac delta functions

For example, consider the one-dimensional functions defined in the range $0 \le x \le L$:

$$f_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi n x}{L}\right)$$

$$\langle f_n(x) | f_{n'}(x) \rangle = \delta_{nn'}$$

For $L \to \infty$ for domain $-\infty \le x \le \infty$

$$\to |f_k(x)\rangle = \sqrt{\frac{1}{2\pi}} e^{ikx}$$

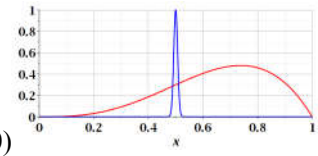
$$\langle f_k(x) | f_{k'}(x) \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(k-k')x} dx = \delta(k - k')$$

Properties of the Dirac delta function

$$\delta(x) = \begin{cases} 0 & \text{for } x \neq 0 \\ \infty & \text{for } x = 0 \end{cases}$$

$$\int_{-\epsilon}^{\epsilon} \delta(x)dx = 1$$

$$\int_{-\infty}^{\infty} G(x)\delta(x)dx = G(0)$$



Properties of the Dirac delta function -- continued

$$\int_{-\infty}^{\infty} G(x)\delta(f(x))dx = \sum_i \frac{G(x_i)}{\left|\frac{df}{dx}\right|_{f(x_i)=0}}$$

$$\int_{-\infty}^{\infty} G(x)\delta'(x)dx = -\left.\frac{dG(x)}{dx}\right|_{x=0}$$