

Function Spaces & Hermitian Operators

Liboff, chap. 4 (3.1)

Now we'll develop some of the mathematical framework, namely Hilbert space & Hermitian operators. Hilbert space will involve the notion of complete sets of functions, and we'll use the solutions for the particle in a box as examples.

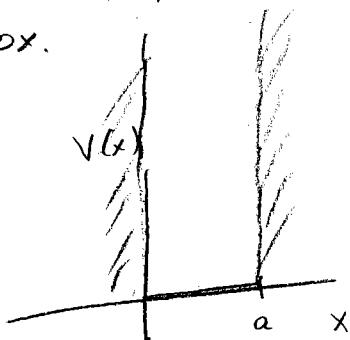
Particle in a box: review

We covered this problem already in P237, so this is just meant to be a review. You should work through this problem in detail (in Liboff, or in your P237 text or notes) to refresh your memory.

Imagine a point mass constrained to move on a thin, frictionless wire strung between two impenetrable walls, a distance a apart. This is a physical picture of a particle in a 1-D box.

Potential is

$$V(x) = \begin{cases} 0 & 0 < x < a \\ \infty & |x| \leq 0, \quad x \geq a \end{cases}$$



Solve time-indep Schr. eq'n to find energy eigenstates.

for $x \leq 0, x \geq a$: $\hat{H}_1 = \frac{\hat{P}^2}{2m} + V_0, \quad V_0 \rightarrow \infty$

$\Rightarrow \psi = 0$ here

There are two ways to see this

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- $\hat{H}_1 \psi = E \psi$; $E + \psi$ finite, so RHS = finite
 \hat{H}_1 infinite, so finite LHS $\Rightarrow \psi = 0$

b. Solve for $\hat{H}_1 = \frac{P^2}{2m} + V_0$, then take $V_0 \rightarrow \infty$

$$x > a, \text{ get } \psi \sim e^{-\kappa x}, \quad \kappa = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$$

$$x < 0 \quad \psi \sim e^{+\kappa x}$$

Now, $V_0 \rightarrow \infty \Rightarrow \kappa \rightarrow \infty \Rightarrow \psi \rightarrow 0$

2) $0 < x < a$

b.c.'s: $\psi_n(0) = \psi_n(a) = 0$

S.E. becomes $\frac{\partial^2 \psi_n}{\partial x^2} + k_n^2 \psi_n, \quad k_n^2 = \frac{2mE_n}{\hbar^2}$

General sol'n is

$$\psi = A \sin k_n x + B \cos k_n x$$

+ boundary conditions give

$$x=0 \Rightarrow B=0$$

$$x=a \Rightarrow A \sin k_n a = 0 \Rightarrow k_n a = n\pi, \quad n=0, 1, \dots$$

(But $n=0$ gives $\psi=0$)

\Rightarrow Integral number of half-wavelengths fit in box.

Normalization:

$$1 = \int_0^a \psi_n^2 dx = A^2 \int_0^a \sin^2\left(\frac{n\pi x}{a}\right) dx$$

$$\text{let } \theta = \frac{n\pi x}{a}$$

$$d\theta = \frac{n\pi}{a} dx$$

$$x=0 \Rightarrow \theta=0 ; \quad x=a \Rightarrow \theta=n\pi$$

$$= \frac{a}{n\pi} A^2 \int_0^{n\pi} \sin^2 \theta d\theta$$

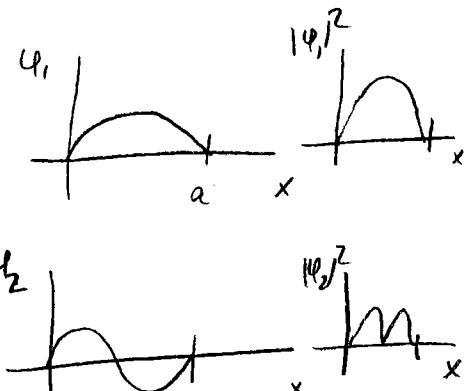
$$\frac{n\pi}{2}$$

$$= \frac{a A^2}{2} \Rightarrow A = \sqrt{\frac{2}{a}}$$

So, for $0 < x < a$,

$$\boxed{\psi_n = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}}$$

$$E_n = \frac{\hbar^2 K_n^2}{2m} = \frac{\hbar^2 \pi^2}{2ma^2} n^2$$



etc

~~+~~

In general, note that a wave function ψ is in general defined only up to an arbitrary phase factor $e^{i\alpha}$. That is, expectation values + the normalization condition only involve ψ^* and ψ together, so $\psi \rightarrow e^{i\alpha} \psi$ does not change the physical results

Bohr Correspondence Principle: When classical \leftrightarrow quantum.

Question: What does the classical probability density look like for this problem (particle in 1D box)?

Answer: Well, we know the particle moves w/ constant velocity (call it v) and between collisions w/ the wall its motion looks like

$$x = x_0 + vt$$

Since the velocity is constant, the particle spends the same amount of time in any given region of fixed size, so the prob. density should be uniform, i.e. constant. To quantify this, note

$P dx = \text{prob of finding particle b/w}$

$$x + x + dx$$

= fraction of time in interval

$$= \frac{dt}{T} \quad + \text{since } T = \frac{a}{v}$$

$$= \frac{v dt}{a}$$

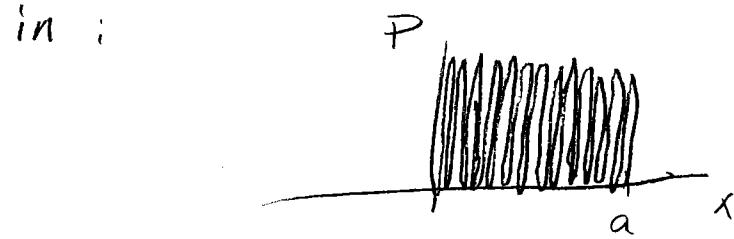
$$= \frac{dx}{a}$$

$$\Rightarrow P = \frac{1}{a} = \text{const}$$

Question: What does the prob. density look like quantum mechanically, and when should it look like the classical one?

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Answer: The first couple prob. densities are shown on p. 3.3 - not terribly uniform! But note that as n increases, more & more peaks get squeezed in:



This is starting to look like a uniform distribution, and for n large enough, it is indistinguishable in practice, because to measure the position of the particle necessarily gives the system a kick (+ hence an uncertainty Δx) that doesn't allow you to distinguish the peaks from the troughs, so the distrib. looks uniform. So in this case, the QM prob approaches the classical prob. for large n .

Bohr correspondence principle: The quantum result for a system or problem must reduce to the corresponding classical result in the classical domain. This domain is the limit where \hbar becomes small (since \hbar doesn't appear in classical mech.) and is often the limit of large quantum numbers.

Dirac Notation

(3.6)

Dirac introduced an elegant notation for use w/
wave functions and integrals involving them.

We will introduce it in the context where we
consider wave functions as explicit functions
of position ("coordinate representation") but
eventually we will see that they have a
much more general usefulness.

Consider the integral of a product of two wave funs

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

In Dirac notation, we write this as

$$\langle \psi | \psi \rangle$$

The whole thing is called a Dirac bracket, and the
parts are the "bra" $\langle \psi |$ and the "ket" $|\psi \rangle$.

As we will see in the next section, the bracket is
equivalent to an inner product on a Hilbert space.

You can think of the ket $|\psi \rangle$ as another
way to write the wave fn.

There's an algebra which goes with all this;
assuming $\langle \psi | \psi \rangle$ is finite, the following properties
hold:

$$\langle \psi | a\psi \rangle = a \langle \psi | \psi \rangle$$

$$\langle a\psi | \psi \rangle = a^* \langle \psi | \psi \rangle$$

→

(3.7)

$$\langle \psi | \psi \rangle^* = \langle \psi | \psi \rangle$$

$$\langle \psi + \psi' | = \langle \psi | + \langle \psi' |$$

$$\int (\psi_1 + \psi_2)^* (\psi_1 + \psi_2) dx = \langle \psi_1 | \psi_1 \rangle + \langle \psi_2 | \psi_1 \rangle + \langle \psi_1 | \psi_2 \rangle + \langle \psi_2 | \psi_2 \rangle$$

+ see book for intermediate steps.

Hilbert space

Now we come to a powerful notion, the idea that eigenstates of an operator can form a vector space.

We'll make an analogy w/ 3-D vectors. We can write a vector \vec{v} as a set of 3 components (v_x, v_y, v_z) , and we can write \vec{v} in terms of three unit vectors $\hat{x}, \hat{y}, \hat{z}$ ($= \hat{i}, \hat{j}, \hat{k}$) which span the space and form a basis:

$$\vec{v} = v_x \hat{x} + v_y \hat{y} + v_z \hat{z}$$

We define an inner product of 2 vectors

$$\vec{v} \cdot \vec{u} = v_x u_x + v_y u_y + v_z u_z$$

+ length is $|\vec{v}| = \sqrt{v_x^2 + v_y^2 + v_z^2}$
Notice that the basis vectors form an orthonormal set, that is their inner product w/ themselves

$$\text{is } 1, \text{ i.e. } \hat{x} \cdot \hat{x} = \hat{y} \cdot \hat{y} = \hat{z} \cdot \hat{z} = 1$$

but they are orthogonal to each other

$$\hat{x} \cdot \hat{y} = \hat{x} \cdot \hat{z} = \hat{y} \cdot \hat{z} = 0$$

Now if we apply the same ideas to functions, we have a space of functions called a Hilbert space. (3.8)

Hilbert space \mathcal{H} :

- Linear: a) $\varphi \in \mathcal{H} \Rightarrow a\varphi \in \mathcal{H}$

- b) $\varphi, \psi \in \mathcal{H} \Rightarrow \varphi + \psi \in \mathcal{H}$

(closed under addition, closed under multiplication by a const.)

- 3 inner product $\langle \varphi | \psi \rangle$, for $\varphi, \psi \in \mathcal{H}$

for functions defined for $a \leq x \leq b$ (1D), e.g.

$$\langle \varphi | \psi \rangle = \int_a^b \varphi^* \psi \, dx$$

- 3 norm $\|\varphi\|$ s.t.

$$\|\varphi\|^2 = \langle \varphi | \varphi \rangle$$

- Completeness: Limit of every Cauchy sequence $\in \mathcal{H}$

[A Cauchy sequence is one w/ diminishing distance between any pair of members of the sequence. For a sequence $\{\varphi_n\}$, for

any $\epsilon > 0$, \exists some point in the sequence (call it $N(\epsilon)$) beyond which the difference between any two terms in the sequence (φ_n and φ_m say) is $< \epsilon$.

i.e., $\forall \epsilon > 0, \exists N(\epsilon)$ w/ $m > N, n > N$, s.t.

$$\|\varphi_m - \varphi_n\| < \epsilon.$$

Or as the book puts it, $\lim_{n,m \rightarrow \infty} \|\varphi_m - \varphi_n\| = 0 \}$

(3.9)

so, roughly, a Cauchy sequence is a sequence of functions ^{in the space} that get closer & closer together, i.e. they approach some limit. For the space to be a Hilbert space, that limit must also be in the space.

Ex The set of functions defined for $0 \leq x \leq a$ with finite norm

$$\|q\|^2 = \int_0^a q^* q dx < \infty \quad \mathcal{H},$$

is a Hilbert space; call it \mathcal{H} ,

Ex The set of square-integrable functions defined for all x is also a Hilbert space, \mathcal{H}_2

$$\|q\|^2 = \int_{-\infty}^{\infty} q^* q dx < \infty \quad \mathcal{H}_2$$

We can extend the notion of orthogonality to functions: $q + q'$ are orthogonal if their inner product is 0;

$(q | q') = \int q^* q' dx = 0$ orthogonal

(Note: I will sometimes refer to the inner product as an "overlap integral")

We can also have a set of functions which spans a space and forms a basis $\{\psi_n\}$. Then any function in the space can be written as a linear comb. of the basis functions.

$$\Psi(x) = \sum_{n=1}^{\infty} a_n \psi_n(x) \quad (*)$$

where we have assumed a discrete basis set (see below for the continuous case).

Ex: For \mathbb{H}_1 , a basis set is the set of eigenfunctions of the particle-in-a-box Hamiltonian *

Basis vectors form an orthogonal set

$$\langle \psi_n | \psi_{n'} \rangle = 0, \quad n \neq n'$$

and if they are properly normalized they form an orthonormal set

$$\boxed{\langle \psi_n | \psi_{n'} \rangle = \delta_{nn'}} \quad \text{orthonormal}$$

where $\delta_{nn'}$ is the Kronecker delta defined by

$$\delta_{nn'} = \begin{cases} 1 & n=n' \\ 0 & n \neq n' \end{cases}$$

* but not necessarily with the boundary conditions

(The orthogonality means that the overlap integral for two different particle-in-a-box eigenfunctions is zero.) (3.11)

Now, given a basis set, we can find the expansion coefficients a_n (see ^{eq'n}(*) on p. 3.10) for any function!

Use Dirac notation:

$$|\psi\rangle = \sum_n a_n |\psi_n\rangle$$

(+ note we use the ket as a shorthand for the fn itself)

Now take $\langle \psi_n |$ + apply from the left (note this is shorthand for taking an integral):

$$\langle \psi_n | \psi \rangle = \sum_n a_n \langle \psi_n | \psi \rangle$$

$$= \sum_n a_n \delta_{nn'}$$

$$= a_{n'}$$

$$\text{So } a_n = \langle \psi_n | \psi \rangle \quad \text{projection of } \psi \text{ onto } \psi_n$$

You've seen examples of this before whenever you dealt with Fourier series.

Delta function orthogonality + \mathcal{H}_2

(3.12)

We saw^{or rather said} that the Hilbert space \mathcal{H} , has as a basis the set of soins for the 1-D particle in a box.

What about \mathcal{H}_2 , the space of functions w/ finite norm over the entire real line, i.e.

$$\int_{-\infty}^{\infty} \psi^* \psi dx < \infty$$

This is a special case for a couple of reasons. We'll use the plane waves e^{ikx} to span this space. They form a continuous rather than a discrete set (follows fr/ the integration going to $\pm\infty$), so the expansion sum will be an integral (see below).

The other reason it's special is that even though the plane waves span the space, they themselves don't belong to it! Why? Infinite norm.

To be a bit more systematic, consider the eigenfs of the momentum operator \hat{P} :

$$\psi_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$$

They form an orthogonal set:

$$\langle \psi_k | \psi_{k'} \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ix(k'-k)} dx = \delta(k'-k)$$

So the inner product/overlap is 0 if the functions

are the same, and infinite otherwise.

(3.13)

so this set doesn't belong to \mathcal{H}_2 , but any function in \mathcal{H}_2 can be expanded in terms of $\{\psi_k\}$. Now the sum over ψ_k is continuous, i.e., it's an integral:

$$\psi(x) \in \mathcal{H}_2 \Rightarrow$$

$$\psi(x) = \int_{-\infty}^{\infty} b(k) \psi_k(x) dk$$

This is a Fourier integral, analogous to a Fourier series expansion. The $b(k)$ are the coefficients, and we find them in analogy to the way we found the a_n in the discrete case; project ψ onto ψ_k . In Dirac notation,

$$|\psi\rangle = \sum_{-\infty}^{\infty} dk' |b(k') \psi_{k'}\rangle$$

so taking $\langle \psi_k |$ acting on ψ

$$\langle \psi_k | \psi \rangle = \underbrace{\int_{-\infty}^{\infty} dk' b(k') \langle \psi_k | \psi_{k'} \rangle}_{\delta(k-k')}$$

$$\delta(k-k')$$

$$= b(k)$$

+ notice that the Dirac notation gives the same thing for the continuous as for the discrete case (compare a_n on bottom of p. 3.11).

Even though the plane waves aren't properly normalized, they form an extremely useful spanning set for H_2 . [^{Aside} If is possible to get a more proper basis set by taking the functions $\psi_k = \frac{1}{\sqrt{a}} e^{ikx}$ in the interval $-a/2 < x < a/2$ + taking $a \rightarrow \infty$.]

(3.14)

Hermitian Operators

Operators corresponding to physical observables must have some special characteristics. Anything we can measure, i.e. any physical observable, must be a real number or set of real numbers, as in the case of vectors (we can't measure complex numbers). But recall that the possible values of the observed quantity are given by the eigenvalues of the corresponding operators. Therefore

Eigenvalues of an operator corresponding to physical observables must be real.

Hermitian operators have this property. A Hermitian operator is one that is its own Hermitian conjugate (= Hermitian adjoint).

What does that mean?

Hermitian adjoint / Hermitian conjugate: This is like a generalization of complex conjugation. (3.15)

We need to define it in the context of a Hilbert space \mathcal{H} . So let \hat{A} be an operator in \mathcal{H} & also $\psi \in \mathcal{H} \Rightarrow \hat{A}\psi \in \mathcal{H}$.

Then the Hermitian adjoint \hat{A}^+ is defined s.t. for two elements $\psi_n + \psi_e$ of \mathcal{H} ,

$$\langle \hat{A}^+ \psi_e | \psi_n \rangle = \langle \psi_e | \hat{A} \psi_n \rangle \quad \text{Hermitian adjoint}$$

\hat{A}^+ is another operator which may or may not be the same as \hat{A} .

Take a simple case where A just corresponds to multiplying by a complex number a . Then

$$\langle a^+ \psi_e | \psi_n \rangle = \langle \psi_e | a \psi_n \rangle \text{ defines } a^+$$

$$= a \langle \psi_e | \psi_n \rangle \text{ because } a \text{ is a const}$$

$$= \langle a^* \psi_e | \psi_n \rangle$$

$\Rightarrow a^* = a^* \Rightarrow$ Hermitian conjugate of a complex number is its complex conjugate

(Note that this means any real number is its own Hermitian conjugate.)

Ex In \mathcal{H}_2 , take

(3.16)

$$\hat{D} = \frac{\partial}{\partial x}$$

To find its Hermitian adjoint we'll integrate by parts:

$$\langle \hat{D}^+ \psi_e | \psi_n \rangle = \langle \psi_e | \hat{D} \psi_n \rangle$$

$$= \int_{-\infty}^{\infty} dx \psi_e^* \frac{\partial}{\partial x} \psi_n$$

$$= \cancel{\psi_e^* \psi_n} \Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \left(\frac{\partial}{\partial x} \psi_e^* \right) \psi_n dx$$

0 since ψ_e, ψ_n must $\rightarrow 0$
as $x \rightarrow \infty$ for finite norm

$$= \int_{-\infty}^{\infty} (-\hat{D} \psi_e^*) \psi_n dx$$

$$= \langle -\hat{D} \psi_e | \psi_n \rangle$$

$$\Rightarrow \hat{D}^+ = -\hat{D}$$

Now back to the definition of a Hermitian operator:
it's its own Hermitian adjoint.

$$\boxed{\hat{A}^+ = \hat{A}}$$

Hermitian operator

which implies

$$\langle \psi_e | \hat{A} \psi_n \rangle = \langle \hat{A} \psi_e | \psi_n \rangle$$

All physical observables correspond to Hermitian operators
(we'll show that their eigenvalues are real below.).

Ex Any real number is a Hermitian op:

3.17

$$\langle \alpha^* \psi_e | \psi_n \rangle = \langle \alpha \psi_e | \psi_n \rangle = \langle \psi_e | \alpha \psi_n \rangle$$

Exercise: You will show in the homework that

$$(\hat{a}\hat{A} + \hat{b}\hat{B})^+ = \hat{a}^* \hat{A}^+ + \hat{b}^* \hat{B}^+$$

and $(\hat{A}\hat{B})^+ = \hat{B}^+ \hat{A}^+$

Q: Suppose $\hat{A} + \hat{B}$ are Hermitian. Is $\hat{A}\hat{B}$ also?

A: $(\hat{A}\hat{B})^+ = \hat{B}^+ \hat{A}^+ = \hat{B}\hat{A}$

which is not the same as $\hat{A}\hat{B}$ necessarily.

(Example: $\hat{A} = \hat{x} + \hat{B} = \hat{P}$. \hat{P} contains a derivative
so $\hat{P}\hat{x}$ isn't necessarily equal to $\hat{x}\hat{P}$.)

Q: Okay, then can we construct a combination of $\hat{A} + \hat{B}$ that is Hermitian? (still assuming $\hat{A}^+ = \hat{A}^* + \hat{B}^* = \hat{B}$)

A: Yes. $(\hat{A}\hat{B} + \hat{B}\hat{A})^+ = \hat{B}^+ \hat{A}^+ + \hat{A}^+ \hat{B}^+ = \hat{B}\hat{A} + \hat{A}\hat{B} = \hat{A}\hat{B} + \hat{B}\hat{A}$
so $\hat{A}\hat{B} + \hat{B}\hat{A}$ is Hermitian if $\hat{A} + \hat{B}$ are.

Q: If \hat{A} is Hermitian, is \hat{A}^2 ?

A: Yep. $(\hat{A}^2)^+ = (\hat{A}\hat{A})^+ = \hat{A}^+ \hat{A}^+ = \hat{A}\hat{A} = \hat{A}^2$

(can also show using defining relation (p.3.15))

Ex: Momentum + Energy Ops: Are they Hermitian? 3.18
 They'd better be, since they correspond to physical
 observables. (Consider H_2 .)

$$\begin{aligned}\hat{P} : \langle \psi_e | \hat{P} \psi_n \rangle &= \int_{-\infty}^{\infty} \psi_e^* (-i\hbar \frac{\partial}{\partial x}) \psi_n dx \\ &= -i\hbar \left[\psi_e^* \psi_n \right]_{-\infty}^{\infty} + i\hbar \int_{-\infty}^{\infty} \left(\frac{\partial}{\partial x} \psi_e^* \right) \psi_n dx \\ &= \int_{-\infty}^{\infty} \left(i\hbar \frac{\partial}{\partial x} \psi_e \right)^* \psi_n dx = \langle \hat{P} \psi_e | \psi_n \rangle\end{aligned}$$

$\therefore \hat{P}$ is Hermitian.

Note we could have gotten this from knowing

$$\hat{D}^+ = -\hat{D} \text{ where } \hat{D} = \frac{\partial}{\partial x}$$

$$\hat{P} = -i\hbar \hat{D} ; \quad \hat{P}^+ = i\hbar \hat{D}^+ = -i\hbar \hat{D} = \hat{P}$$

\hat{H} , free particle:

$$\hat{H} = \frac{\hat{P}^2}{2m} \Rightarrow \hat{H}^+ = \left(\frac{\hat{P}}{2m} \right)^+ = \frac{(\hat{P}^2)^+}{2m} = \frac{\hat{P}^2}{2m}$$

\hat{H} , with potential: $V(x)$ is just a real function that multiplies ψ , so it is Hermitian also:

$$\begin{aligned}\langle \psi_e | V \psi_n \rangle &= \int_{-\infty}^{\infty} \psi_e^* V \psi_n dx = \int_{-\infty}^{\infty} V \psi_e^* \psi_n dx \\ &= \int (V \psi_e)^* \psi_n dx = \langle V \psi_e | \psi_n \rangle\end{aligned}$$

Properties of Hermitian Operators

(3.19)

We brought up Hermitian operators because we said physical observables must be real, so we need operators w/ real eigenvalues, ^{and such ops} are Hermitian. Now we'll show that Hermitian operators have real eigenvalues and orthogonal eigenfunctions.

① Hermitian operators have real eigenvalues.

Hermitian operator \hat{A} , eigenvalues $\{a_n\}$ + eigenfns $\{\psi_n\}$

$$\hat{A}\psi_n = a_n\psi_n$$

or in Dirac notation

$$|\hat{A}\psi_n\rangle = |a_n\psi_n\rangle \text{ or } \hat{A}|\psi_n\rangle = a_n|\psi_n\rangle$$

Take inner prod. w/ $|\psi_n\rangle$

$$\langle\psi_n|\hat{A}\psi_n\rangle = \langle\psi_n|a_n\psi_n\rangle = a_n\langle\psi_n|\psi_n\rangle \quad (= a_n \text{ if } \psi_n \text{ normalized})$$

But LHS is also, since \hat{A} is Hermitian, equal to

$$\text{LHS} = \langle\hat{A}\psi_n|\psi_n\rangle = \langle a_n\psi_n|\psi_n\rangle = a_n^* \langle\psi_n|\psi_n\rangle$$

$$\Rightarrow a_n = a_n^*$$

② The eigenfunctions of Hermitian op's are orthogonal

Take

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

* mult. on left by $\langle\psi_1|$

(3.2)

$$\Rightarrow \langle \psi_e | \hat{A} | \psi_n \rangle = a_n \langle \psi_e | \psi_n \rangle$$

but we also have since \hat{A} is Hermitian

$$\text{LHS} = \langle \hat{A} | \psi_e | \psi_n \rangle = a_e^* \langle \psi_e | \psi_n \rangle = a_e \langle \psi_e | \psi_n \rangle$$

Now subtract the two eq'n's \Rightarrow

$$(a_e - a_n) \langle \psi_e | \psi_n \rangle = 0$$

which means, if $a_e \neq a_n$ (nondegenerate),

$$\langle \psi_e | \psi_n \rangle = 0$$

So if the ψ_n are properly normalized,

$$\langle \psi_e | \psi_n \rangle = 0$$

Comment: Suppose you have an operator \hat{A} . You can always write it as a linear combination of Hermitian and antihermitian ($\hat{B}^+ = -\hat{B}$; note $\frac{\partial}{\partial x}$ is antih hermitian) ops;

$$\hat{A} = \underbrace{\frac{\hat{A} + \hat{A}^+}{2}}_{\text{Herm.}} + \underbrace{\left(\frac{\hat{A} - \hat{A}^+}{2} \right)}_{\text{anti-hermit}}$$