

# LITTLEJOHN QUANTUM MECHANICS

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Notes for Littlejohn's Quantum Mechanics course (Physics 221AB) at UC Berkeley during Fall 2020 and Spring 2021. All materials (including lecture videos) for the course are being posted online so I thought I'd help myself. If you have any comments let me know at [hi@delonshen.com](mailto:hi@delonshen.com).

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# LECTURE FROM AUGUST 27, 2020

February 11, 2021

Oh no, the first 20 minutes are missing :( Lets read the lecture notes first then

## THE MISSING 20 MINUTES?

We'll start by defining Hilbert spaces.

**DEFINITION 1: (HILBERT SPACE)** A function  $\psi(x)$  is considered normalizable or square integrable if

$$\int |\psi(x)|^2 < \infty$$

We'll define a Hilbert space as the vector space of complex square integrable functions. It's not too hard to see it satisfies the normal properties of vector spaces so we won't do that here. One thing to note about Hilbert spaces is that they are infinite dimensional.

We know that for a wave function  $\psi(x)$  the norm  $|\psi(x)|^2$  corresponds to the probability density of finding a particle at some position in space. We can relate  $\psi(x)$  to a momentum wave function  $\phi(p)$  via a fourier transform

$$\phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int dx \exp\{-ips/\hbar\} \times \psi(x)$$

The fourier transform is invertible and linear meaning that we have a bijection between the Hilbert space of position wave functions and the space of momentum wave functions. We have from the *Parseval identity* that

$$\int dx |\psi(x)|^2 = \int dp |\phi(p)|^2$$

This means that the space of momentum wave functions contains normalizable functions as well and thus is itself a Hilbert space.

Lets consider the a orthonormal set of eigenfunctions  $u_n$  of some hamiltonian  $H$ . We can expand a wave functions in terms of these eigenfunctions

$$\psi(x) = \sum_i c_i u_i(x) \text{ where } c_i \in \mathbb{C}$$

From orthonormality we can extract the coefficients in the normal way

$$c_i = \int dx u_i^*(x) \psi(x)$$

We can now consider a space  $\{(c_1, c_2, \dots)\}$  of coordinate represntations of the position wave function expanded on a basis of energy eigenstates. By looking at the above expansion we

can intuit that the probability of finding a wavefunction with energy  $E_i$  will be  $|c_i|^2$  (assuming  $\sum_i |c_i|^2 = 1$ .) By orthonormality we also have

$$\int dx |\psi(x)|^2 = \int \left| \sum_i c_i u_i(x) \right|^2 = \sum_i |c_i|^2 \underbrace{\int |u_i(x)|^2}_{1 \text{ by orthonormality}} + \sum_{i \neq j} c_i c_j^* \underbrace{\int u_i(x) u_j^*(x)}_{0 \text{ by orthonormality}} = \sum_i |c_i|^2$$

Thus we can see that the vector space  $\{(c_1, \dots)\}$  is a Hilbert space as well.

None of the Hilbert spaces we've discussed so far is more fundamental, they just correspond to measuring different observables.  $\psi(x)$  helps us measure the position of a wave function,  $\phi(p)$  lets us measure momentum, and  $\{(c_1, \dots)\}$  helps us measure energy. The way we should think about different wave functions is as some state vector on an abstract vector space. The different Hilbert spaces we've observed so far are just projections of that state vector in an abstract vector space to the basis of energy, momentum, etc.

The first postulate of quantum mechanics we'll explore is the idea that any physical system is associated with a complex vector space  $\mathcal{E}$ .  $\mathcal{E}$  can be finite or infinite dimensional depending on the system. Vectors in  $\mathcal{E}$  are represented by ket vector  $|\psi\rangle$ . A pure state of the system can be associated with a one dimensional subspace of  $\mathcal{E}$ . Now let's talk about bras.

From our undergraduate quantum mechanics class we know that  $\langle\psi|$  is the complex conjugate of  $\psi$ . But here we don't want to talk about wave functions (we'll derive those from our abstract vector space construction in the future.) Instead we'll construct  $\langle|$  vectors as a vector in the dual space of  $\mathcal{E}$  which we'll denote as  $\mathcal{E}^*$ .  $\mathcal{E}^*$  will contain complex valued linear functions acting on  $\mathcal{E}$ . A specific instantiation of  $\mathcal{E}^*$  we'll denote as  $\langle\alpha| : \mathcal{E} \rightarrow \mathbb{C}$ . From here we have the usual notation of  $\langle\alpha|\psi\rangle$  that we should be familiar with. It's not too hard to prove that  $\mathcal{E}^*$  is a vector space with the same dimension of  $\mathcal{E}$ .

Now let's ask ourselves how we'll move from ket to bra space. Just like in general relativity we'll need to define a metric (or an inner product). What we're postulating is the existence of some map  $g$  on  $\mathcal{E}$  where

$$g : \mathcal{E} \times \mathcal{E} \rightarrow \mathbb{C}$$

A useful analogy to keep in mind when thinking about this is the euclidean metric which allows us to define distances between points on some flat space. This geometric intuition will be useful in our abstract complex vector space. We'll require that  $g$  is linear in its **second slot** and antilinear in its **first slot**. Concretely this means that

$$g(|\psi\rangle, c_1 |\phi_1\rangle + c_2 |\phi_2\rangle) = c_1 g(|\psi\rangle, |\phi_1\rangle) + c_2 g(|\psi\rangle, |\phi_2\rangle)$$

$$g(c_1 |\phi_1\rangle + c_2 |\phi_2\rangle, |\psi\rangle) = c_1^* g(|\phi_1\rangle, |\psi\rangle) + c_2^* g(|\phi_2\rangle, |\psi\rangle)$$

We'll require that  $g$  is symmetric ( $g(|\psi\rangle, |\phi\rangle) = g(|\phi\rangle, |\psi\rangle)^*$ ) and that  $g$  is positive definite

$$g(|\psi\rangle, |\psi\rangle) \geq 0 \text{ where equality only occurs when } |\psi\rangle = 0$$

Now using this metric we can define the dual correspondance  $DC : \mathcal{E} \rightarrow \mathcal{E}^*$  by defining a bra's  $\langle\psi|$  action on an arbitrary ket vector as

$$\langle\psi|\phi\rangle = g(|\psi\rangle, |\phi\rangle)$$

From the properties of the metric we see that the bra  $\langle\psi|$  is a map  $\mathcal{E} \rightarrow \mathbb{C}$  and that the space of bra vectors form a vector space. For notation we'll denote the bra associated with a  $|\psi\rangle$  as  $\langle\psi| = (|\psi\rangle)^\dagger$ . Since the metric is antilinear in its first argument we find that the dual correspondance (taking the hermitian conjugate) is antilinear as well

$$(c_1|\psi\rangle + c_2|\phi\rangle)^\dagger = c_1^* \langle\psi| + c_2^* \langle\phi|$$

We'll move onto proving an important inequality for complex vector space, the Schwarz inequality

$$|\langle\psi|\phi\rangle|^2 \leq \langle\psi|\psi\rangle \langle\phi|\phi\rangle$$

Before we continue lets try to use our geometrical intuition from euclidean space to get some intuition. The above statement is equivlant to saying in euclidean space for two vectors **a** and **b**

$$\langle \mathbf{a}, \mathbf{b} \rangle^2 \leq |\mathbf{a}|^2 |\mathbf{b}|^2 \Rightarrow \langle \frac{\mathbf{a}}{|\mathbf{a}|}, \frac{\mathbf{b}}{|\mathbf{b}|} \rangle \leq 1$$

What the inequality is saying is that if you project a vector onto some direction then it will never exceed its original length. From this reframing we can also say that equality only happens if we project the vector along the direction it's already pointing in. In other words equality only happens if **a** and **b** lie on the same ray. Now lets go back to our complex bra and ket space case and prove it for our situation. Consider

$$|\alpha\rangle = |\psi\rangle + \lambda|\phi\rangle \Rightarrow \langle\alpha|\alpha\rangle = \langle\psi|\psi\rangle + \lambda^* \langle\phi|\psi\rangle + \lambda \langle\psi|\phi\rangle + |\lambda|^2 \langle\phi|\phi\rangle \geq 0$$

From here let

$$\lambda = -\frac{\langle\phi|\psi\rangle}{\langle\phi|\phi\rangle} \Rightarrow \langle\psi|\psi\rangle - \frac{|\langle\psi|\phi\rangle|^2}{\langle\phi|\phi\rangle} > 0 \Rightarrow \langle\psi|\psi\rangle \langle\phi|\phi\rangle \geq |\langle\psi|\phi\rangle|^2$$

Lets move on.

**DEFINITION 2: (LINEAR OPERATORS)** A linear operator  $L : \mathcal{E} \rightarrow \mathcal{E}$  maps vectors in ket space to vectors in ket space. They have all the usual properties you know and love. The commutator of two linear operators  $A$  and  $B$  is

$$[A, B] = AB - BA$$

**DEFINITION 3: (LIE ALGEBRA)** If some bracket operations defined on some hilbert space satisfy the following properties then we can classify the vector space as a lie algebra

$$[c_1 A_1 + c_2 A_2, B] = c_1 [A_1, B] + c_2 [A_2, B]$$

$$[A, c_1 B_1 + c_2 B_2] = c_1 [A, B_1] + c_2 [A, B_2]$$

$$[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0$$

<sup>1</sup>I don't think I've understood the dual correspondance very well.

A useful feature of hilbert spaces is that they always have a countable basis. Consider on such basis  $\{|n\rangle, n = 1, 2, \dots\}$ . For an arbitrary state vector  $|\psi\rangle$  we can expand it in terms of this basis

$$|\psi\rangle = \sum_n c_n |n\rangle$$

An orthornomal basis has the following properties

$$\langle n|n\rangle = 1 \Rightarrow c_n = \langle n|\psi\rangle$$

This gives us another useful property about the outer product of  $|n\rangle$

$$|\psi\rangle = \sum_n c_n |n\rangle = \left( \sum_n |n\rangle \langle n| \right) |\psi\rangle \Rightarrow \sum_n |n\rangle \langle n| = 1$$

### BACK TO THE LECTURE

We want to choose some notation that doesn't doesn't prefer some Hilbert space. We'll do this by introducing a hilbert space called the ket space

$$\text{state space} = \mathcal{E} = \{|\psi\rangle\}$$

This state space is isomorphic to all the hilbert spaces we've discussed above. What we do to go from state space to the hilbert spaces we've talked about before is that we choose some basis and project some state vector to the basis we desire. The basis we choose are usually associated with some physical observable. This is the basic idea of wave functions we'll talk about. Since we're talking about ket space lets talk about the postualtes of quantum mechanics. The first postulate is that any physical statement corresponds to some hilbert space  $\mathcal{E}$ . the properties of this Hilbert space is determined by the proeptries of the physcial systems. Another postulate is that a *pure state* corresponds to a ray  $\subset \mathcal{E}$ .

**DEFINITION 4: (RAY)** A one dimensional vector subspace of our state space  $\mathcal{E}$ .

$$\text{Ray} = \{|\psi\rangle = c|\psi_0\rangle | |\psi_0\rangle \neq 0, c \in \mathbb{C}\}$$

The vectors of the ray only differ from the fundamental "Vector" that defines the way by an arbitrary prefactor. Sometimes we'll say "the state" blah blah blah and we'll write down a vector but we don't mean that the vector is state but we really mean the ray

So the move is to work with ket spaces instead of wave functions(and only use wave functions to callback our old experience.)

Despite working as a programmer for five year Prof. Littlejohn hates modern technology. Okay lets talk about ket spaces. One thing we know how to do is take complex conjugates of wave functions. But how do we complexconjugate kets? They're not numbers so we can't take a complex conjugate. We can do this by using a dual correspondance and defining a dual space. If we have a vector space  $\mathcal{E}$  then we can define a dual space that contains maps of  $\mathcal{E} \rightarrow \mathbb{C}$ . We know these things as bra  $\langle\alpha|$ .

**DEFINITION 5: (BRA)** A **bra** is a linear map

$$\langle \alpha | : \mathcal{E} \rightarrow \mathbb{C}$$

This means that

$$\langle \alpha | (|\psi\rangle) = \text{complex number}$$

Linearity is

$$\langle \alpha | (c_1 |\psi\rangle + c_2 |\phi\rangle) = c_1 \langle \alpha | (|\psi\rangle) + c_2 \langle \alpha | (|\phi\rangle)$$

If we want to find the sum of two bras we just find the action of the sum on some arbitrary ket

$$(\langle \alpha | + \langle \beta |)(|\psi\rangle) = \langle \alpha | (|\psi\rangle) + \langle \beta | (|\psi\rangle)$$

Similarly we have

$$(c \langle \alpha |)(|\psi\rangle) = c[\langle \alpha | (|\psi\rangle)]$$

A dual space like this is defined for any vector space we can think of.

**DEFINITION 6: (DUAL SPACE)**

$$\text{dual space} = \mathcal{E}^* = \{\langle \alpha | \text{ acting on } \mathcal{E}\}$$

The dual space is infinite dimensional if  $\mathcal{E}$  is infinite dimensional and same for finite dimensional.

Now we need to define a map  $DC : \mathcal{E} \rightarrow \mathcal{E}^*$  which we call the dual correspondance. To find the dual correspondance we need to talk about a metric. This is basically defining a inner product for our vector space.

**DEFINITION 7: (METRIC)** A **metric** on a space  $\mathcal{E}$  is a map denoted by  $g$

$$g : \mathcal{E} \times \mathcal{E} \rightarrow \mathbb{C}$$

We require some things from the metric

(a)  $g$  is linear in 2nd operand

$$g(|\psi\rangle, c_1 |\phi\rangle + c_2 |\alpha\rangle) = c_1 g(|\psi\rangle, |\phi\rangle) + c_2 g(|\psi\rangle, |\alpha\rangle)$$

(b)  $g$  is anti-linear in the first operand

$$g(c_1 |\psi\rangle + c_2 |\phi\rangle, |\alpha\rangle) = c_1^* g(|\psi\rangle, |\alpha\rangle) + c_2^* g(|\phi\rangle, |\alpha\rangle)$$

(c) Symmetry

$$g(|\psi\rangle, |\phi\rangle) = g(|\phi\rangle, |\psi\rangle)^*$$

(d) Positive-definite

$$g(|\psi\rangle, |\psi\rangle) \geq 0 \quad \forall |\psi\rangle \text{ where equality happens iff } |\psi\rangle = 0$$

So we can use the metric to obtain the dual correspondance which is the mapping from ket to bra.

$$g(\underbrace{|\psi\rangle}_{\text{fixed}}, \underbrace{|\phi\rangle}_{\text{variable}})$$

Since  $g$  is linear in the second operand what we have is a linear operand that acts on some ket and outputs a bra vector. This means that this map is a bra vector

$$g(|\psi\rangle, |\phi\rangle) = \langle\psi|(|\phi\rangle)$$

This is our dual correspondance and the definition of  $\langle\psi|$ . For finite dimensional vector this dual correspondance is bijective. Okay so lets make notational changes to make our lives much nicer

- (a) We'll drop the parenthesis when we write the action of bras on kets  $\langle\psi|(|\phi\rangle) \rightarrow \langle\psi|\phi\rangle = g(|\psi\rangle, |\phi\rangle)$
- (b)  $\langle\psi|\phi\rangle = \langle\phi|\psi^*\rangle$
- (c)  $\langle\psi|\psi\rangle \geq 0$  where equality only occurs when  $|\psi\rangle = 0$
- (d)  $\langle\psi| = |\psi\rangle^\dagger$

The dual correspondance is invertible in Hilbert so daggering something twice is just the identity map. e.g.

$$\langle\psi|^\dagger = |\psi\rangle \Rightarrow |\psi\rangle^{\dagger\dagger} = |\psi\rangle$$

The schwarz inequality is

$$|\langle\psi|\phi\rangle|^2 \leq \langle\psi|\psi\rangle\langle\phi|\phi\rangle$$

This is important since it's used to derive the uncertainty principle.

Lets talk about linear and anti-linear operators.

$$\text{Linear } L : \mathcal{E} \rightarrow \mathcal{E} \quad \text{Antilinear } A : \mathcal{E} \rightarrow \mathcal{E}$$

The difference between the two is that

$$L(c_1|\psi\rangle + c_2|\phi\rangle) = c_1L|\psi\rangle + c_2L|\phi\rangle \quad A(\dots) = c_1^*A|\psi\rangle + c_2^*A|\phi\rangle$$

The only antilinear operator that important in this course is the time reversal operator. For now lets forget antilinear operators and assume from now on that everything is a linear operator. Here's some things we can say. We can multiply them

$$A(BC) = (AB)C$$

Composition of maps (products of operators) is associative.

$$AB \neq BA \quad [A, B] = AB - BA$$

The commutator has a lot of properties we remember from undergrad. One thing to mention is that commutator in QM is closely related to poisson bracket in CM.

Given a linear operator  $A$  where  $A|\psi\rangle$  we can define another operator  $\tilde{A} : \mathcal{E}^* \rightarrow \mathcal{E}^*$ . What's the action of this on a bra?

$$\langle\psi|\tilde{A} \quad ((\langle\psi|\tilde{A})(|\phi\rangle) = \langle\psi|(A|\phi\rangle))$$

We get tired writing the tilde so we just leave off the tilde. But once we've done that we realize that the parenthesis don't matter so we can rewrite the above as a "matrix element"

$$\langle\psi|A|\phi\rangle$$

So that's the action of operators on bras

If we have kets  $\alpha$  and  $\beta$  then we define the outer product of  $\alpha$   $\beta$  as

$$\text{Outer Product } |\alpha\rangle\langle\beta|$$

This means we can define a linear operator

$$(|\alpha\rangle\langle\beta|)(|\psi\rangle) = |\alpha\rangle\langle\beta|\psi\rangle$$

Now lets talk a bit from basis. In any vector we know what a basis is. This also applies to Hilbert space. However Hilbert spaces may be infinite dimensional. So we might ask if the basis is countable (exists bijection to natural numbers?) The answer is that the mathematical structure of Hilbert spaces is that they always have a set of countable basis. This doesn't mean we'll always use the countable basis. In fact we frequently don't use the countable basis. But for right now we should keep in mind that for any space of wave function we can choose a countable basis. Alright lets suppose we have some ket space  $\mathcal{E}$  with a countable basis  $\{|n\rangle\}$ . We have the normal definition of orthonormality

$$\langle n|m\rangle = \delta_{mn}$$

Alright if we have this then we can take an arbitrary state  $|\psi\rangle$  so that

$$|\psi\rangle = \sum_n |n\rangle c_n$$

By doing the normal orthogonality method we have  $c_n = \langle n|\psi\rangle$ . So now we have an expression

$$|\psi\rangle = \left( \sum_n |n\rangle\langle n| \right) |\psi\rangle \Rightarrow \text{Resolution of Identity } \sum_n |n\rangle\langle n| = 1$$

Now we should talk a bit about Hermitian conjugation which maps kets to bras and bras to kets. We'll also define these on complex numbers where hermitian conjugation is just complex conjugation. Finally we'll define complex conjugation on operators as follows

$$A : \mathcal{E} \rightarrow \mathcal{E} \Rightarrow A^\dagger : \mathcal{E} \rightarrow \mathcal{E} \text{ such that } A^\dagger|\psi\rangle = (\langle\psi|A)^\dagger$$

Littlejohn's learning so much about iPad cameras today. There's a whole bunch of properties that follow from above

$$\langle\psi|A^\dagger|\phi\rangle^* = \langle\phi|A|\psi\rangle \quad (|\alpha\rangle\langle\beta|)^\dagger = |\beta\rangle\langle\alpha| \dots$$

Basically you reverse the result and dagger everything. Now we can define hermitian operators



**DEFINITION 8: (HERMITIAN/ANTI-HERMITIAN/UNITARY OPERATORS)** An operator  $A$  is **hermitian** if  $A^\dagger = A$ , **anti-hermitian** if  $A^\dagger = -A$ , and **unitary** if  $U^\dagger = U^{-1}$

We'll blow off a lot the functional analysis for QM here. Some books on this would be Reed and Simon's book. We'll get by in this course with just intuition. Lets talk about eigenvalues and eigenkets

$$\underbrace{\text{if } A |u\rangle}_{\text{eigen-ket}} = \underbrace{a}_{\text{right eigenvalue}} |u\rangle \quad |u\rangle \neq 0 \quad c \in \mathbb{C}$$

And something similar for eigenbra and "left" eigenvalues. Now lets talk about the spectrum of operators

$$\text{Spectrum of } A = \{c \in \mathbb{C} | A|u\rangle = c|u\rangle \text{ where } |u\rangle \in \mathbb{E} \neq 0\}$$

If we take a hermitian operator  $A$  then the spectrum consists completely of real numbers. If  $A$  is unitary then we have a spectrum that lies on the unit circle in the complex plane. So that's the meaning of the spectrum of the operator. The case of hermitian operators is the most special one.

**DEFINITION 9: (EIGENSPACE)** If we write the eigenket equation

$$A|u\rangle = a|u\rangle$$

Lets let  $a_n \in \text{Spectrum of } A$ . Then we'll define the **eigenspace**  $\mathcal{E}_n$  as

$$\mathcal{E}_n = \{|u\rangle \in \mathbb{E} | A|u\rangle = a_n|u\rangle\} \subset \mathcal{E}$$

This has dimensionality of at least one. Furthermore if we have an infinite dim hilbert space then we can have infinite dimensional eigenspaces as well (e.g. parity operator has two eigenspaces, even and odd functions, that are both infinite dimensional). If  $\dim \mathcal{E} = 1$  then it's **non-degenerate** and if  $> 1$  then its **degenerate**

Consider an hermitian operator  $A$ . We know that  $A$  has the following properties

- (a) Eigenvalues of real
- (b) Eigenbra = dagger eigenket
- (c) Eigenspaces corresponding to distinct eigenvalues are orthogonal. Lets provethis. Consider

$$A|u\rangle = a|u\rangle \quad A|u'\rangle = a'|u'\rangle \Rightarrow \langle u'|A|u\rangle = a\langle u'|u\rangle \text{ and } \langle u|A|u'\rangle = a'\langle u|u'\rangle$$

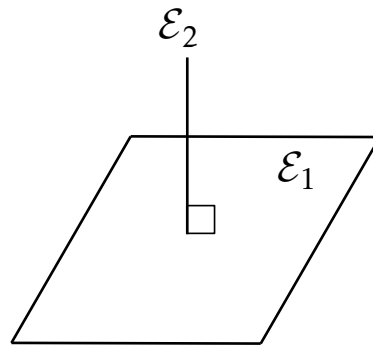
Now taking the complex conjugate of the final relation gives us

$$\langle u'|A|u\rangle = a'\langle u'|u\rangle$$

Now equating everything we get

$$(a - a')\langle u'|u\rangle = 0 \Rightarrow \text{Either } a = a' \text{ or } \langle u|u'\rangle = 0$$

A picture of this is below



when we have a hermitian operator we have real eigenvalues and orthogonal eigenspaces. The eigenkets are normalizable since they belong to a Hilbert space. One thing we can ask is if the eigenspaces fill out the entire space or do they leave some corners left out. If they do then the operator is called **complete**. If the operator is complete then we can choose an eigenbasis. But what if they don't fill out the space? Well when we do not consider hermitian operators then its usually the case that operators are not complete. Consider

$$\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$$

**In finite dimensions all operators are complete.** In infinite dimensions this is not necessarily true. In infinite dimensions this problem becomes more complicated because of the continuous spectrum. Lets introduce this today. Consider a wave function  $\psi(x)$ . Let  $\hat{p}$  be the momentum operator with eigenvalues  $p$ . The momentum operator is defined as

$$(\hat{p}\psi)(x) = -i\hbar \frac{d\psi}{dx}$$

So now we can find the eigenfunctions of the momentum operator denoted by  $u_p$

$$(\hat{p}u_p)(x) = pu_p(x) = -i\hbar \frac{d}{dx}u_p(x) \Rightarrow u_p(x) = e^{\frac{ipx}{\hbar}}$$

So what we can say is in finite dimensions the eigenvalues of hermitian operators are always real. If  $p$  has a imaginary part then the function diverges as we go to  $-\infty$  or  $\infty$  so it's not normalizable. If  $p$  is only real then we have a oscillatory function which still isn't normalizable. So how do we interpret this? We can deal with this by saying the eigenvalues are a continous spectrum. He's out of time so we'll continue with this next time.

## LECTURE FROM SEPTEMBER 01, 2020

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### MORE FORMALISM

Recall the spectral properties of operators we had from last lecture. We know that a hermitian operator is complete meaning we have an orthonormal eigenbasis

$$A|nr\rangle = a_n|nr\rangle$$

Where  $r$  is the degeneracy of the eigenvalue  $a_n$ . We have

$$\langle n' r' | nr \rangle = \delta_{nn'} \delta_{rr'}$$

By the resolution of the identity we have

$$1 = \sum_{n,r} |nr\rangle \langle nr| = \sum_n P_n$$

Where  $P_n$  is the projection operator onto  $\mathcal{E}_n$

$$P_n = \sum_r |nr\rangle \langle nr|$$

Tonight we'll discuss how this nice picture changes when we go to infinite dimension spaces. Consider the harmonic oscillator

$$H|n\rangle = E_n|n\rangle \text{ where } E_n = n + \frac{1}{2}$$

Where we have a discrete spectrum. Things generalize naturally to infinite dimensions here. Now consider the momentum operator  $\hat{p} = -i\hbar d/dx$  where we call this a q-number while  $p$  is the eigenvalue is a c-number. We have

$$\hat{p}u_p(x) = pu_p(x) = -i\hbar \frac{d}{dx}u_p(x) \Rightarrow u_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{ipx}{\hbar}}$$

If we restrict  $p \in \mathbb{R}$  we have a continuous spectrum. We have

$$\langle p|p'\rangle = \int dx u_p(x)^* u_{p'}(x) = \delta(p - p')$$

Where **red term** is what allowed things to have a nice normalization. It also turns out that the eigenfunctions are complete.

$$1 = \int dp |p\rangle \langle p|$$

So we have a complete orthonormal basis if we allow basis that lie outside of Hilbert space and have normalization of the basis vector in a delta function sense.

Lets look at another example,  $\hat{x}$  and  $x$  the c-number. We have

$$\hat{x}u_{x_0}(x) = xu_{x_0}(x) \Rightarrow u_{x_0}(x) = \delta(x - x_0)$$

This has the orthonormality relation

$$\langle x_0|x_1\rangle = \delta(x_0 - x_1)$$

These are normalized in the delta function sense just like the momentum eigenfunctions. We also have

$$1 = \int dx |x\rangle \langle x|$$

**EXAMPLE 1: (HYDROGEN ATOM)** The usual energy eigenfunctions have eigenkets  $|nlm\rangle$  giving us

$$H|nlm\rangle = E_n|nlm\rangle \text{ where } E_n = -\frac{1}{2n^2}$$

We have an orthonormal eigenstates

$$\langle nlm|n'l'm'\rangle = \delta_{nn'}\delta_{ll'}\delta_{mm'}$$

These are only the bound states and these states don't have a resolution of the identity

$$1 \neq \sum_{nlm} |nlm\rangle\langle nlm|$$

We also need to include states with positive energy.

$$H|Elm\rangle = E|Elm\rangle \text{ where } E \in \mathbb{R}^+$$

These are normalized in a delta function

$$\langle Elm|E'l'm'\rangle = \delta(E - E')\delta_{ll'}\delta_{mm'}$$

To complete the orthonormality relation we also need

$$\langle nlm|El'm'\rangle = 0$$

In any case we have the resolution of identity as

$$1 = \sum_{nlm} |nlm\rangle\langle nlm| + \int_0^\infty dE \sum_{lm} |Elm\rangle\langle Elm|$$

There does exist a projection operator to the bound states

$$P_n = \sum_{lm} |nlm\rangle\langle nlm|$$

The **blue term** might also look like a projection operator but it turns out it isn't and we'll talk about that later. The hydrogen atom is an example of a mixed spectrum

Lets consider some general cases. In infinite dimensions we say that **complete hermitian operators are observables** (remember not all hermitian operators are complete in infinite dimensions). In this course all hermitian operators we'll consider are complete. So we'll just assume that any hermitian operator we encounter is complete. Anyways some more general notation

$$A|nr\rangle = a_n|nr\rangle \text{ a discrete spectrum where } r \text{ is the degeneracy}$$

$$A|vr\rangle = a(v)|vr\rangle \text{ a continuous spectrum}$$

We write the orthonormality relations as

$$\langle nr|n'r'\rangle = \delta_{nn'}\delta_{rr'} \quad \langle nr|vr'\rangle = 0 \quad \langle vr|v'r'\rangle = \delta(v - v')\delta_{rr'}$$

Then the general form of the resolution of identity is

$$1 = \sum_{nr} |nr\rangle\langle nr| + \int dv \sum_r |vr\rangle\langle vr|$$

We have some projection operator

$$P_n = \sum_r |nr\rangle\langle nr|$$

Does  $|vr\rangle\langle vr|$  form a projection operator? No. However consider some interval  $I = [v_0, v_1]$ . Then we have

$$P_I = \int_I dv \sum_r |vr\rangle\langle vr|$$

For a concrete example of this let's consider the momentum operator

$$P_I = \int_{p_0}^{p_1} dp |p\rangle\langle p|$$

This is like Fourier transforming our space wave function and throw away everything outside the interval. This is like how filters work in the real world.

Let's talk about function of operators. First we'll define

$$f(A) = \sum_{nr} a_n |nr\rangle\langle nr| + \int dv a(v) \sum_r |vr\rangle\langle vr|$$

We can also define more exotic function

$$f(A) = \frac{1}{x - A}$$

TODO: I think I've missed something here.

Let's talk a bit more about projectors.

**DEFINITION 10: (PROJECTORS)** A projector  $P$  is an observable such that

$$P^2 = P \text{ idempotent}$$

This means that the eigenvalues have

$$p^2 = p \Rightarrow p = 0, 1$$

Thus we have two orthogonal eigenspaces  $\mathcal{E}_0$  and  $\mathcal{E}_1$ . The 0 eigenstate is the annihilation of some dimension and the 1 eigenstate is the projection onto some dimension.

Now let's consider more than one observable  $A$  and  $B$ .  $A$  and  $B$  (posses simultaneous eigenbasis) iff they commute. To show this (in one direction) let's talk about invariant subspaces

**DEFINITION 11: (INVARIANT SUBSPACE)** Let  $\mathcal{S} \subset \mathcal{E}$ .  $\mathcal{S}$  is invariant under  $A$  if the action of  $A$  brings vectors of  $\mathcal{S}$  to vectors in  $\mathcal{S}$

$$|\psi\rangle \in \mathcal{S} \rightarrow A|\psi\rangle \in \mathcal{S}$$

This means we can define a hermitian operator  $\bar{A} : \mathcal{S} \rightarrow \mathcal{S}$ .

Lets assume  $A$  and  $B$  commute. Consider the eigenspaces of  $A$   $\mathcal{E}_{1,2}$ . These eigenspaces of invariant subspaces.

$$|\psi\rangle \in \mathcal{E}_n \rightarrow A|\psi\rangle = a_n|\psi\rangle \in \mathcal{E}_n$$

The restricted operator  $\bar{A} = a_n \bar{I}_d = a_n$ . What we're saying is the restricted operator is a constant. It turns out that if  $A$  commutes with  $B$  then the eigenspace also belongs to  $b$ . Suppose  $|\psi\rangle \in \mathcal{E}_n$ . Then we have

$$A|\psi\rangle = a_n|\psi\rangle$$

Now what about  $AB|\psi\rangle$ ? Well we can write

$$A(B|\psi\rangle) = BA|\psi\rangle = a_n B|\psi\rangle$$

Since acting with  $A$  on  $B|\psi\rangle$  brings out  $a_n$  which is associated with  $\mathcal{E}_n$  we can say that  $B|\psi\rangle \in \mathcal{E}_n$  and thus the eigenspace  $\mathcal{E}_n$  is also invariant under  $B$ . This means that we have a restricted operator  $\bar{B} : \mathcal{E}_n \rightarrow \mathcal{E}_n$  which is a hermitian operator on  $\mathcal{E}_n$  meaning that we have an eigenbasis on this space  $|nr\rangle$  so that  $B|nr\rangle = b_{nr}|nr\rangle$ . These are eigenvectors of  $B$  in  $\mathcal{E}_n$ . If we do this on all eigenspaces of  $A$  then we have two orthonormal eigenbasis for  $A$  and  $B$ .

Here's another theorem that has a lot of applications. Lets  $A$  and  $B$  be observables and assume that they commute. Lets also assume we have a nondegenerate  $A|\psi\rangle = a|\psi\rangle$ . We then have some  $B|\psi\rangle = b|\psi\rangle$  for some  $b$ . The reason fro this is

$$A(B|\psi\rangle) = BA|\psi\rangle = a(B|\psi\rangle)$$

This says that  $B|\psi\rangle$  is in the non-degenerate eigenspace of  $a$  and thus  $B|\psi\rangle = b|\psi\rangle$  since  $|\psi\rangle$  is the only dimension  $B|\psi\rangle$  could be along given the constraints. We'll now move onto a different set of topics.

## POSTULATES OF QUANTUM MECHANICS

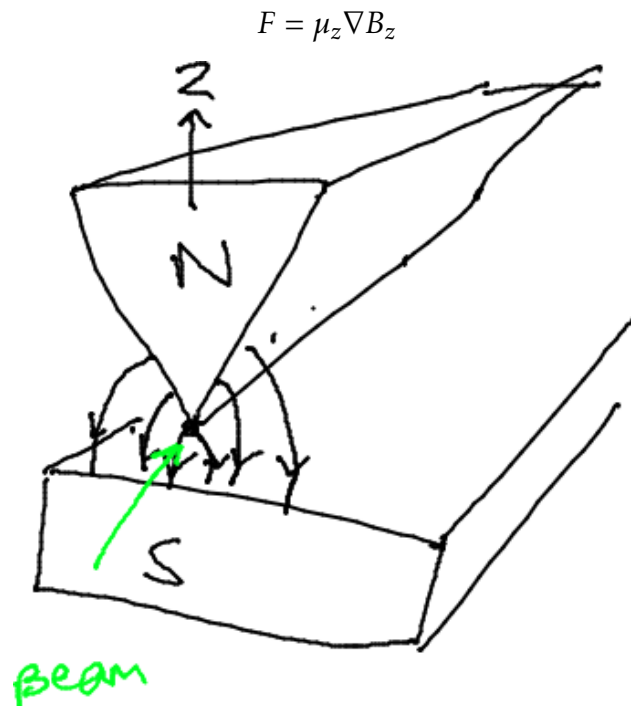
Lets now talk about the postulates of quantum mechanics.

- (a) Every physical systems corresponds to a hilbert space  $\mathcal{E}$ .
- (b) A pure state of the system is a ray in  $\mathcal{E}$ . (a pure state is a state where we have the maximum amount of information about it.) We talk about a  $|\epsilon\rangle$  Ray as a representative element in the ray
- (c) Every measurement process on the system corresponds to an observable  $A$  where  $A : \mathcal{E} \rightarrow \mathcal{E}$ .
- (d) possible outcomes of measurements are equal to the eigenvalues of the observable  $A$  (in the discrete case it's the  $a_n$  or in the continuous case is  $a(\nu)$ )

- (e) The probability of measuring  $(A = a_n) = \langle \psi | P_n | \psi \rangle / \langle \psi | \psi \rangle$ . and similarly for the continuous case the probability of measuring  $(a_0 \leq A \leq a_1) = \langle \psi | P_I | \psi \rangle / \langle \psi | \psi \rangle$  where  $I = [a_0, a_1]$
- (f) After a measurement  $|\psi\rangle \mapsto P_n |\psi\rangle$  or similarly  $|\psi\rangle \mapsto P_I |\psi\rangle$ . (collapse)

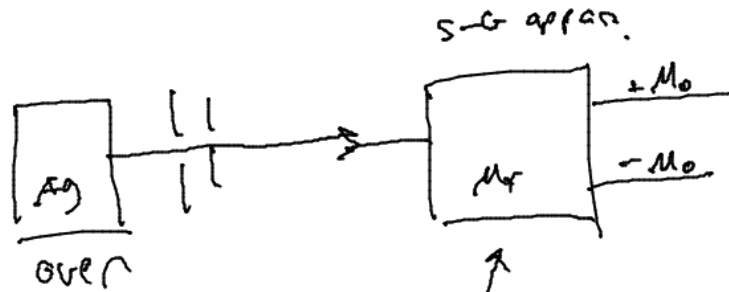
There are things we should say. Postulate (5) is stated in terms of probability. So what this is implying is that QM is not telling us what an outcome is but rather a probability distribution of possible outcomes. Probabilities are determined by making a measurement of an ensemble of similarly prepared experiments. The important thing of all of this is that some state vector  $|\psi\rangle$  is not an individual system but an ensemble of similarly prepared systems. What collapse is saying is that we reduce our ensemble  $|\psi\rangle$  to a smaller ensemble  $P|\psi\rangle$ .

**EXAMPLE 2: (STERN-GERLACH EXPERIMENT)** Let's measure the magnetic moment of a particle. We have a classical picture of the magnetic moment (precessing dipole.) TODO classical picture. tldr



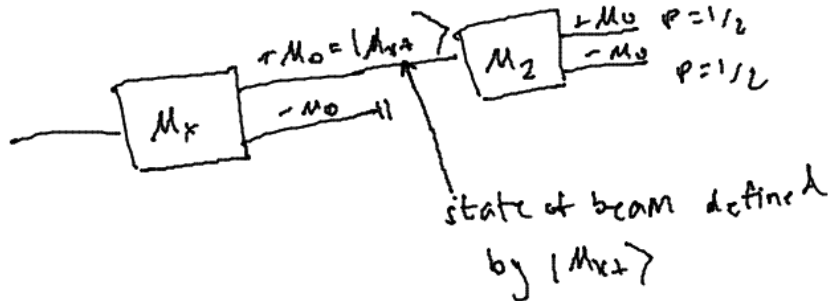
Let's assume that the dipole moment is equal in magnitude and  $\mu_z = \mu_0 \cos \theta$ . With just classical mechanics is that there's a continuum between two dots. However S-G observed two spots with no continuum. This is regarded as space quantization.

Now let's pretend that we know nothing except the postulates of QM. We know that Ag is neutral but has a magnetic moment.



postulate says  $\exists \mathcal{E}$  with at least  $\dim=2$  since two possible outcomes

$\dim \mathcal{E}=2$   
Basis  $|\mu_{x+}\rangle, |\mu_{x-}\rangle$  (or  $\psi, z \Rightarrow 3$  possible basis.



Now let's expand (where  $|\pm\rangle = |\mu_{z\pm}\rangle$ )

$$|\mu_{x+}\rangle = c_+|+\rangle + c_-|-\rangle \Rightarrow \langle \pm | \mu_{x+} \rangle = c_{\pm}$$

We know that

$$p(\mu_z = +\mu_0) = \frac{1}{2} = \langle \mu_{x+} | P_+ | \mu_{x+} \rangle \text{ where } P_+ = |+\rangle \langle +|$$

This allows us to write

$$p(\mu_z = \mu_0) = \langle \mu_{x+} | + \rangle \langle + | \mu_{x+} \rangle = |c_+|^2$$

We can generically write a normalized coefficient

$$c_+ = \frac{e^{i\alpha_1}}{\sqrt{2}} \quad c_- = \frac{e^{i\beta_1}}{\sqrt{2}} \Rightarrow |\mu_{x+}\rangle = \frac{1}{\sqrt{2}} (e^{i\alpha_1} |+\rangle + e^{i\beta_1} |-\rangle)$$



If we change the phase we get  $|\mu_{x+}\rangle = |\mu_{x+}\rangle e^{i\alpha_1}$  thus giving us

$$|\mu_{x+}\rangle = \frac{1}{\sqrt{2}}(|+\rangle + e^{i\beta_1} |-\rangle)$$

Where there's one unknown coefficient  $\beta_1$ . Similarly we can get

$$|\mu_{x-}\rangle = \frac{1}{\sqrt{2}}(|+\rangle + e^{i\gamma_1} |-\rangle)$$

We can fix these phases by using  $\langle\mu_{x+}|\mu_{x-}\rangle = 0$  and this gives us  $e^{i\gamma_1} = -e^{-i\beta_1}$  meaning that

$$|\mu_{x\pm}\rangle = \frac{1}{\sqrt{2}}(|+\rangle \pm e^{i\beta_1} |-\rangle)$$

We can similarly find

$$|\mu_{y\pm}\rangle = \frac{1}{\sqrt{2}}(|+\rangle \pm e^{i\gamma_1} |-\rangle)$$

This is building up the state vectors (and similarly the operators) of the system.

## LECTURE FROM SEPTEMBER 03, 2020

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In the case of a discrete spectrum we can write  $A = \sum_n a_n P_n$ . In the case of  $\mu_x$  we can write

$$\mu_x = \mu_0 |\mu_{x+}\rangle \langle\mu_{x+}| - \mu_0 |\mu_{x-}\rangle \langle\mu_{x-}|$$

If we plug in our result from last time we can write

$$\mu_x = \frac{\mu_0}{2} \left\{ (|+\rangle + e^{i\beta_1} |-\rangle)(\langle+| + e^{-i\beta_1} \langle-|) - (|+\rangle - e^{i\beta_1} |-\rangle)(\langle+| - e^{-i\beta_1} \langle-|) \right\} = \mu_0 \left[ e^{i\beta_1} |-\rangle \langle+| + e^{-i\beta_1} |+\rangle \langle-| \right]$$

And we can do a similar calculation to get

$$\mu_y = \mu_0 \left[ e^{i\gamma_1} |-\rangle \langle+| + e^{-i\gamma_1} |+\rangle \langle-| \right]$$

$$\mu_z = \mu_0 [(|+\rangle \langle+|) - (|-\rangle \langle-|)]$$

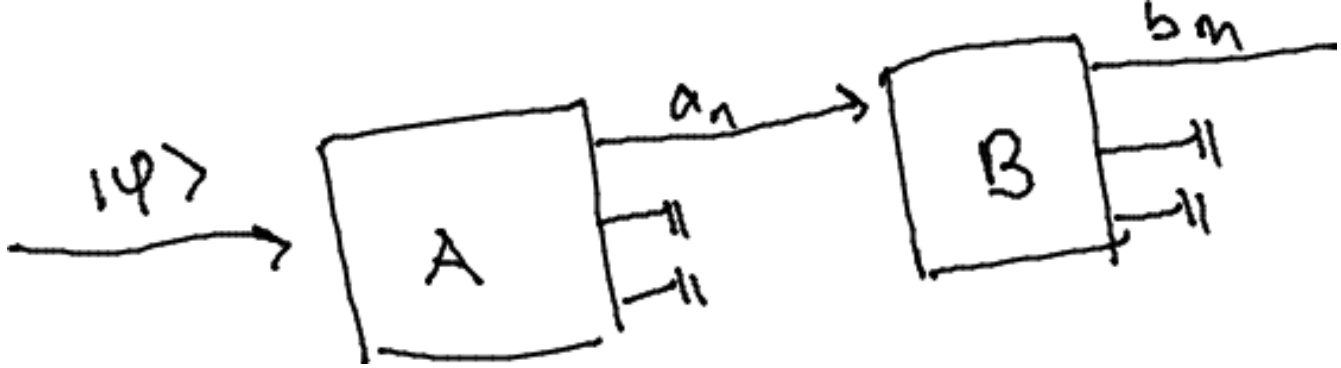
So what about these phases? Lets go back and instead of feeding the positive  $\mu_x$  into  $\mu_z$  lets feed positive  $\mu_x$  into  $\mu_y$ . This gives

$$|\langle\mu_{x+}|\mu_{y+}\rangle|^2 = \frac{1}{2} = \left| \frac{1}{2} \left( (|+\rangle + e^{-i\beta_1} \langle-|)(|+\rangle + e^{i\gamma_1} |-\rangle) \right) \right|^2 \Rightarrow \cos(\gamma_1 - \beta_1) = 0 \Rightarrow \gamma_1 = \beta_1 \pm \pi \Rightarrow e^{i\gamma_1} = \pm i e^{i\beta_1}$$

Something to note is that the **red term** implies whatever we do we'll have imaginary matrix elements. We're gonna make the  $\mu_x$  real and  $\mu_y$  imaginary. We can then write

$$\mu_x = \mu_0 \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \mu_y = \pm \mu_0 \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad \mu_z = \mu_0 \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

So this is an example where we can use the postulates of quantum mechanics to create the operators that result in measurements in quantum mechanics. There's one more loose end we need to tie up. We assumed that the eigenspaces of  $\mu_{x,y,z}$  are nondegenerate. So how do we know about degeneracy? To do this let's consider measurement processes from a more general standpoint.



We want to find that

prob of measuring  $b_m$  after first measuring  $a_n = p(a_n; b_m) = \frac{\langle \psi | P_{A_n} | \psi \rangle}{\langle \psi | \psi \rangle} \times \frac{\langle \psi_1 | P_{B_m} | \psi_1 \rangle}{\langle \psi_1 | \psi_1 \rangle}$  where  $\psi_1 = P_{A_n} | \psi \rangle$

$$\text{note that } \langle \psi_1 | \psi_1 \rangle = \langle \psi | \underbrace{P_{A_n}^\dagger P_{A_n}}_{P_{A_n}} | \psi \rangle = \langle \psi | \psi \rangle \Rightarrow p(a_n; b_m) = \frac{\langle \psi | P_{A_n} P_{B_m} P_{A_n} | \psi \rangle}{\langle \psi | \psi \rangle}$$

If we do the reverse experiment

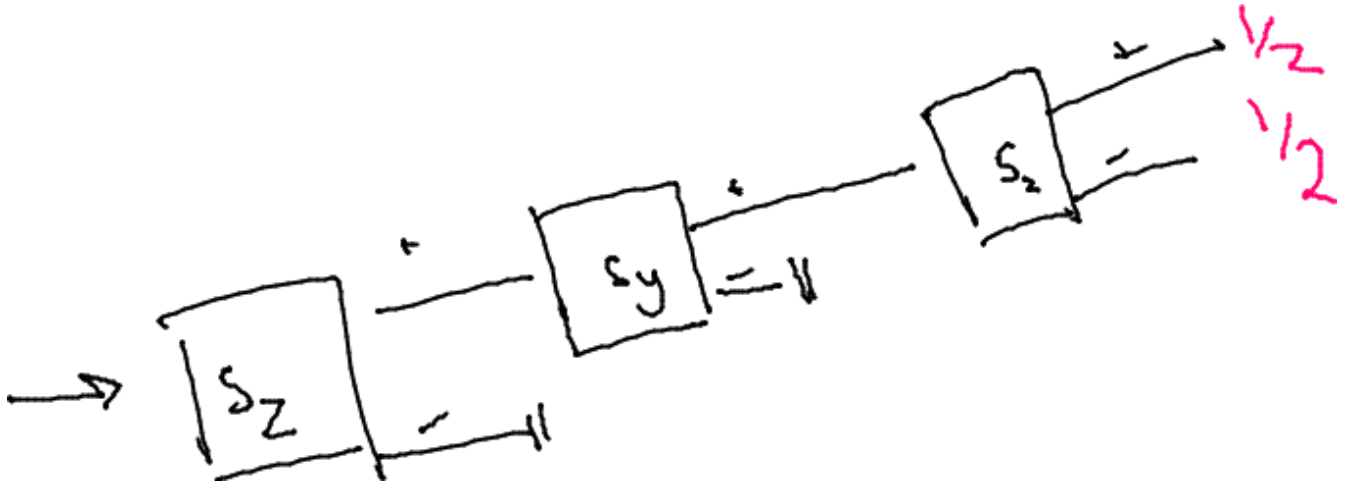
$$p(b_m; a_n) = \frac{\langle \psi | P_{B_m} P_{A_n} P_{B_m} | \psi \rangle}{\langle \psi | \psi \rangle} \neq p(a_n; b_m)$$

On the other hand if  $[A, B] = 0$  then we can show that  $[P_{A_n}, P_{B_m}] = 0$  and this is because these are functions of the operators. The converse is true. What this means is that the probabilities are the same. So we could determine the commutivity of operators by doing experiments in reverse. Now suppose we find an operator  $B$  that commutes with  $A$ . We have a state  $\psi_1$  that is in the eigenspace of  $A_n$ . Now when we measure again with  $B$  what we're doing is projection  $\psi_1$  onto a subspace of  $A_n$ . Also note that the eigenspace that corresponds to  $b_m$  and  $b'_m$  must be orthogonal by nature. So that means if our measurement of  $B$  results in multiple outputs from  $\psi_1$  then we know the dimensions of the eigenspace of  $A_n > 1$  due to the orthogonality of the subeigenspaces of the  $b_m$ . **So we can determine the degeneracy of some eigenspace of  $A$  if we can find another operator  $B$  which commutes with  $A$  that can resolve the degeneracy like we did above.** We can keep doing this, e.g. find an observable  $C$  that commutes with  $A$  and  $B$  and can measure the simultaneous eigenspace corresponding to  $A_n$  and  $B_m$ . How do we know where to stop? In principle we don't.

**DEFINITION 12: (COMPLETE SET OF COMMUTING OBSERVABLES)** A set of commuting observables which implies that they have simultaneous eigenspaces. A CSCO has all non-degenerate eigenspaces.

In practice we'll treat the electron wave function as a scalar even though we have spin (another commuting observables.) This is an example where we don't consider the full CSCO. So that's the story of resolving identities and observables. Lets go back to non-commuting observables.

To get a more extreme version of the difference between classical and quantum statics lets consider the Stern-Gerlach experiment again.



What's going on with the last probabilities? It's not what we'd expect with classical statistics.

Lets consider a classical system with a classical hamiltonian  $h(q, p)$ . Now lets say we have some apparatus with classical hamiltonian  $H(Q, P)$  that measures thing. Then we have

$$H_{\text{tot}} = h(q, p) = H(Q, P)$$

Now lets say we ant to measure  $q_1$  from  $h$ . Then we need to introduce an interaction that depends on  $q_1$

$$H_{\text{tot}} = h(q, p) = H(Q, P) + I(q_1, Q, P)f(t)$$

Where  $f(t)$  is a function that determines when the measurement takes place(smearing function?). So what happens to the  $Q$  variables evolution

$$\dot{Q} = \frac{\partial H}{\partial P} + \frac{\partial I}{\partial P}f(t) \text{ and } \dot{P} = -\left(\frac{\partial H}{\partial Q} + \frac{\partial I}{\partial Q}f(t)\right)$$

Where the blue terms are the interaction terms. What about

$$\dot{q}_1 = \frac{\partial H_{\text{tot}}}{\partial p_1} = \frac{\partial h}{\partial p_1} \text{ and } \dot{p}_1 = -\frac{\partial H_{\text{tot}}}{\partial q_1} = -\frac{\partial h}{\partial q_1} - \frac{\partial I}{\partial q_1}f(t)$$

So what we see here is that  $p_1$  has some perturbative evolution from the measurement. So this isn't exactly classical statistics (balls and bins) since you'lll introduce perturbation when you do measurements. In the case of the SG experiment if we consider a magnetic pole in some magnetic field we'll have the pole precess. So if we measure  $s_z$  the  $s_x$  and  $s_y$  are moving. In classical mechanics we could in principle compensate by solving the equations of motion to deterine the rate of precession. However you don't do that in quantum mechanics because of

the uncertainty principle. There are a few more things we can say about measuring. Lets say we take the average of some observable

$$\langle A \rangle = \langle a \rangle = \sum_n \text{prob}(a_n) \times a_n = \sum_n \langle \psi | p_n | \psi \rangle a_n = \langle \psi | A | \psi \rangle$$

And in a similar way we can calculate dispersions

$$\Delta A^2 = \Delta a^2 = \sum_n \text{prob}(a_n) (a_n - \langle A \rangle)^2 = \langle \psi | (A - \langle A \rangle)^2 | \psi \rangle$$

Let's also talk about the generalized uncertainty principle. Consider  $A$  and  $B$  which are observables. Let  $\Delta A^2$  and  $\Delta B^2$  be dispersions (variance)

$$\Delta A^2 \Delta B^2 \geq \frac{1}{4} |\langle [A, B] \rangle|^2$$

Where we average wrt some  $|\psi\rangle$ . Lets make some comments before we make a proof. The  $\psi$  is some ensemble. This is not taking some member of the ensemble, measuring the dispersion of  $A$  and then measuring the dispersion of  $B$ . That's something completely different. The most famous version of this is

$$\Delta x^2 \Delta p^2 \geq \frac{\hbar^2}{4} \Leftrightarrow \Delta x \Delta p \geq \frac{\hbar}{2}$$

Let's now proof this with the schwarz inequality. Let  $A_1 = A - \langle A \rangle$  and  $B_1 = B - \langle B \rangle$ . Also define  $|\alpha\rangle = A_1 |\psi\rangle$  and  $|\beta\rangle = B_1 |\psi\rangle$ . If we do this then

$$\Delta A^2 = \langle \alpha | \alpha \rangle = \langle \psi | A_1^2 | \psi \rangle$$

So what we have is

$$\Delta A^2 \Delta B^2 = \langle \alpha | \alpha \rangle \langle \beta | \beta \rangle \geq |\langle \alpha | \beta \rangle|^2$$

Where the final inequality comes from the schwarz inequality. Lets look more closely at the final expression

$$\langle \alpha | \beta \rangle = \langle \psi | A_1 B_1 | \psi \rangle = \underbrace{\frac{1}{2} \langle \psi | [A_1, B_1] | \psi \rangle}_{\text{pure imaginary}} + \underbrace{\frac{1}{2} \langle \psi | \{A_1, B_1\} | \psi \rangle}_{\text{pure real}}$$

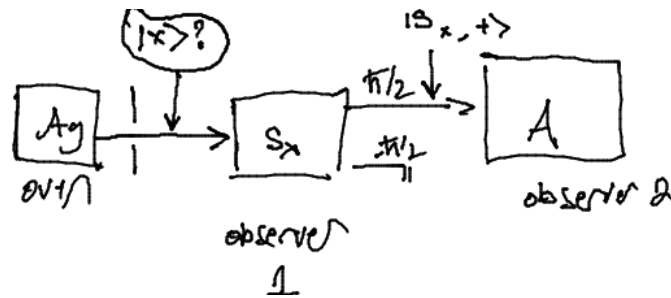
Commutators of hermitian operators are antihermitian and expectation values of anti-hermitian are purely imaginary. Anticommutators of hermitian are hermitian. So if we mode square thing we have

$$|\langle \alpha | \beta \rangle|^2 = \frac{1}{4} \left( |\langle \psi | [A_1, B_1] | \psi \rangle|^2 + |\langle \psi | \{A_1, B_1\} | \psi \rangle|^2 \right) \geq \frac{1}{4} |\langle \psi | [A_1, B_1] | \psi \rangle|^2$$

And since  $\langle A \rangle$  and  $\langle B \rangle$  are c-numbers they commute with everything and thus we have

$$\Delta A^2 \Delta B^2 \geq \frac{1}{4} |\langle \psi | [A, B] | \psi \rangle|^2$$

Lets go back to the Stern-Gerlach experiment



So what is

$$\langle A \rangle = \langle S_x, + | A | S_x, + \rangle$$

But what about  $|\chi\rangle$ ? Does there exist a state vector that describes  $|\chi\rangle$ ? No, and the reason for this is that the expectation value of the spin operator is zero for all three spin operators

$$\langle S_{x,y,z} \rangle = 0 \Rightarrow \langle \mathbf{S} \rangle = 0$$

We know it has to be this way because if it wasn't then there would be some privileged direction of spin which shouldn't happen in the case of thermal equilibrium in the oven with silver atoms. On the other hand if the beam was described by some beam  $|\chi\rangle$  then the expectation value of spin would definitely not be zero.

$$|\chi\rangle = \alpha|+\rangle + \beta|-\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \text{ where } |\alpha|^2 + |\beta|^2 = 1$$

And with these we'd find that

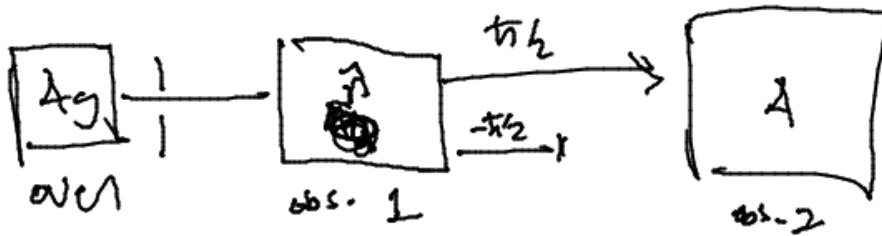
$$\langle \chi | \mathbf{S} | \chi \rangle = \frac{\hbar}{2} \underbrace{\begin{bmatrix} 2\text{Re}(\alpha^*\beta) \\ 2\text{Im}(\alpha^*\beta) \\ |\alpha|^2 - |\beta|^2 \end{bmatrix}}_{\hat{\mathbf{n}}} = \frac{\hbar}{2} \hat{\mathbf{n}}$$

If we write  $\hat{\mathbf{n}} = (\theta, \phi)$  then we have

$$\chi = \begin{bmatrix} e^{-i\phi/2} \cos \frac{\theta}{2} \\ e^{i\phi/2} \sin \frac{\theta}{2} \end{bmatrix} \Rightarrow \langle \chi | \mathbf{S} | \chi \rangle = \begin{bmatrix} \sin \theta \cos \phi \\ \sin \theta \sin \phi \\ \cos \theta \end{bmatrix}$$

All of this is to say that the beam cannot be described by a state vector. So how do we describe

the beam ensemble with no state vector? Lets do a bizzare experiment



choos random direction in sphere  $\hat{n}$

obs. makes sg. apparatus  
to align with  $\hat{n}$ .

Then obs. 2 will have  $\langle \vec{S} \rangle = 0$   
unpolarized (b/f observer 1) and  
randomly polarized (after observer 1)  
ensembles are equivalent

So if we do this then

$$\langle A \rangle = \frac{1}{4\pi} \int d\Omega \langle \hat{n} \cdot (\mathbf{S}, +) | A | \hat{n} \cdot (\mathbf{S}, +) \rangle$$

Where we understand  $\hat{n}$  as oriented in the direction of the solid angle which is what we're integrating over. So we're taking the expectation value as if we knew what the polarization was and averaging over all polarizations. So the beam is modelled by a statistical ensemble of state vectors.

Lets talk about statistical ensembles of state vectors from a more general point of view. Consider some parameters  $\lambda = (\lambda_1, \dots)$ . For example  $(\theta, \phi)$ . Furthermore we have a probability distribution

$$f(\lambda) \geq 0 \text{ where } \int d\lambda f(\lambda) = 1$$

Furthermore we have state vector  $|\psi(\lambda)\rangle$ . Now we have

$$\langle A \rangle = \int d\lambda f(\lambda) \langle \psi(\lambda) | A | \psi(\lambda) \rangle$$

We might also have discrete distribution of state vector. Lets have

$$|\psi_i\rangle \leftrightarrow f_i \text{ where } f_i \geq 0, \sum_i f_i = 1$$

The  $|\psi_i\rangle$  don't have to be orthogonal nor do they have to be a basis. However we will assume that they are normalized  $\langle\psi_i|\psi_i\rangle = 1$ . Then we have

$$\langle A \rangle = \sum_i f_i \langle\psi_i|A|\psi_i\rangle$$

This is the discrete case of statistical ensemble of state vectors. To encompass both these cases we introduce the density operator

**DEFINITION 13: (DENSITY OPERATOR)**

$$\rho = \begin{cases} \sum_i f_i |\psi_i\rangle\langle\psi_i| & \text{discrete} \\ \int d\lambda f(\lambda) |\psi(\lambda)\rangle\langle\psi(\lambda)| & \text{continuous} \end{cases}$$

We can then write the expectation value as

$$\langle A \rangle = \text{tr}(\rho A)$$

To illustrate this in the discrete case

$$\text{tr}(\rho A) = \text{tr}\left(\sum_i f_i |\psi_i\rangle\langle\psi_i| A\right) = \sum_i f_i \text{tr}\left(\underbrace{\langle\psi_i|A|\psi_i\rangle}_{\text{matrix element}}\right) = \sum_i f_i \langle\psi_i|A|\psi_i\rangle = \langle A \rangle$$

This gives the outcome of an arbitrary measurement in the case when we're dealing with a general statistical ensemble of state vectors. This in fact gives us the result of a measurement of an arbitrary measurement on a system. It isn't obvious that this is the result of a general measurement since it's in terms of an expectation value. Suppose we have an operator  $A$  with a discrete spectrum  $\{a_n, p_n\}$  we'd measure eigenvalues. If we're a bit loose we can have  $\langle P_n \rangle = p_n$  and thus  $\langle P_n A \rangle = p_n a_n$ . So what we might say is that  $\rho$  contains all the information on some ensemble. The converse is that we can determine  $\rho$  with measurements. By some miracle we also find that  $\rho$  is unique. Alright now then..... that's the density operator.

**DEFINITION 14: (PURE STATE)** The density operator  $\rho$  is a pure state if there exists some  $|\psi\rangle$  (which we interpret as the wave function) such that

$$\rho = |\psi\rangle\langle\psi|$$

If a state is not pure then it is called mixed which has no wave function

Lets look at some properties of the density operator.

- (a) The density operator is hermitian.  $\rho = \rho^\dagger$ .
- (b) The trace of  $\rho$  is one.  $\text{tr } \rho = \sum_i f_i \langle \psi_i | \psi_i \rangle = 1$ . This is really a statement of the normalization of probability
- (c) We know that  $\rho \geq 0$ , it's a non-negative definite operator. What this means is that

$$\langle \phi | \rho | \phi \rangle = \sum_i f_i \langle \phi | \psi_i \rangle \langle \psi_i | \phi \rangle = \sum_i f_i |\langle \phi | \psi_i \rangle|^2 \geq 0 \quad \forall \phi$$

There's an interesting calculation that we'll try to do today. Let's go back to the thermal beam which is coming from the oven. Based on what we know we have

$$\rho = \frac{1}{4\pi} \int d\Omega |\hat{\mathbf{n}} \cdot \mathbf{S}+\rangle \langle \hat{\mathbf{n}} \cdot \mathbf{S}+|$$

If we explicitly insert the form of  $\hat{\mathbf{n}}$  (in terms of angles on Bloch spheres) what we get is

$$\rho = \frac{1}{4\pi} \int d\Omega \begin{bmatrix} \cos^2 \theta/2 & e^{-i\phi} \sin \theta/2 \cos \theta/2 \\ \text{c.c} & \sin^2 \theta/2 \end{bmatrix}$$

When we average over solid angles we find the diagonal elements vanish (because of exponential) so we're left with

$$\rho = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix}$$

So this is the density matrix of the thermal beam coming from the oven. So there's an interesting thing. Let's go back to our picture.



obs. 1 flip in

$+$   $\rightarrow$  polarized in  $+z$   
 $-$   $\rightarrow$  polarized in  $-z$

In this case

$$\rho = \frac{1}{2} |+\rangle \langle +| + \frac{1}{2} |-\rangle \langle -| = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix}$$

This is exactly what we had before. What this saying is that these two ensembles are exactly the same. What this example illustrates is that a given density operator can be decomposed into multiple different pure states.

## SOME PROBLEMS FROM MATHEMATICAL FORMALISM NOTES

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## PAULI MATRICES

First recall the Pauli matrices

$$I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

The first thing we want to do is show that

$$\sigma_i \sigma_j = \delta_{ij} + i\epsilon_{ijk} \sigma_k$$

Which is pretty quickly confirmed with mathematica. This allows us to quickly derive

$$[\sigma_i, \sigma_j] = 2i\epsilon_{ijk} \sigma_k \quad \{\sigma_i, \sigma_j\} = 2\delta_{ij}$$

Now lets consider two vectors of operators  $A_a$  and  $B_b$  as well as the pauli vector  $\sigma_c$ . If  $[A_i, \sigma_j] = 0$  and  $[B_i, \sigma_j] = 0$  we want to show that

$$(\sigma^i A_i)(\sigma^j B_j) = A^i B_i + i\sigma^i (\epsilon_{ijk} A^j B^k)$$

*Proof.* I think it might come back to bite me in the ass for trying to be fancy and use index notation since the usual arbitrary ordering of things in index notation doesn't apply here because these are operator values vectors and operators in general don't commute. We'll see how it goes though. We'll start by considering the **left hand side**. First since  $\sigma$  and  $A$  commute we can write

$$\text{lhs} = A_i \sigma^i \sigma^j B_j$$

Now we use the commutation of  $\sigma_i \sigma_j$  to get

$$(\text{Left hand side}) = A_i (\sigma^j \sigma^i + 2i\epsilon^{ijk} \sigma_k) B_j$$

$$(\text{using relation confirmed with mathematica}) = A_i (\delta^{ij} + i\epsilon^{jik} \sigma_k + 2i\epsilon^{ijk} \sigma_k) B_j$$

$$(\text{antisymmetry of levi-civita}) = A_i (\delta^{ij} i\epsilon^{ijk} \sigma_k) B_j$$

$$(\text{contract indices}) = A_i B^i + i(\epsilon^{ijk} A_i B_j) \sigma_k \quad \square$$

The next thing we want to show is that for an arbitrary unit vector  $n^i$  and angle  $\theta$  we can write

$$\exp\{-i\theta \sigma^i n_i\} = \cos \theta - i(\sigma^i n_i) \sin \theta$$

*Proof.* Lets start expanding

$$(\text{left hand side}) = 1 - i\theta \sigma^i n_i - \frac{1}{2!} \theta^2 (\sigma^i n_i)^2 + \frac{i}{3!} \theta^3 (\sigma^i n_i)^3 + \dots$$

Now notice that

$$(\sigma^i n_i)^2 = (\sigma^i n_i \times \sigma^j n_j) = n_i n_j \sigma^i \sigma^j = n_i n_j (\delta^{ij} + i\epsilon^{ijk} \sigma_k) = \underbrace{n_i n^i}_1 + i n_i n_j \sigma_k \epsilon^{ijk}$$

Now notice since  $n_i n_j$  are constants they commute and this implies the **green term vanishes**.

$$\begin{aligned}
 \text{green stuff} &= i n_i n_j \sigma_k \epsilon^{ijk} \\
 (\text{relabel dummies}) &= i n_j n_i \sigma_k \epsilon^{jik} \\
 (\text{commutation of scalars}) &= i n_i n_j \sigma_k \epsilon^{jik} \\
 (\text{antisymmetry of levi-civita}) &= -i n_i n_j \sigma_k \epsilon^{ijk} \\
 \Rightarrow (\text{green stuff}) &= 0 \Rightarrow (\sigma_i n_i)^2 = 1 (\text{or technically identity I guess})
 \end{aligned}$$

So we now have

$$(\text{left hand side}) = 1 + i\theta \sigma^i n_i - \frac{1}{2!} \theta^2 + \frac{i}{3!} \theta^3 (\sigma^i n_i) + \dots$$

And it just becomes a matter of reading off the series expansion of sin and cos

$$\exp\{-i\theta \sigma^i n_i\} = \cos \theta - i \sigma^i n_i \sin \theta$$

□

### A LITTLE BIT OF LIE ALGEBRA

(a) The first thing we want to show is that for two arbitrary operators  $A$  and  $B$

$$e^A B e^{-A} = B + [A, B] + \frac{1}{2!} [A, [A, B]] + \frac{1}{3!} [A, [A, [A, B]]]$$

*Proof.* We're given the hint to consider

$$F(\lambda) = e^{\lambda A} B e^{-\lambda A}$$

Now we can expand in powers of  $\lambda$  to get.

$$\begin{aligned}
 F(\lambda) &= \left(1 + A\lambda + \frac{A^2 \lambda^2}{2} + \dots\right) B \left(1 - A\lambda + \frac{A^2 \lambda^2}{2} - \dots\right) \\
 &= (B + AB\lambda + \frac{AAB\lambda^2}{2} + \dots)(1 - A\lambda + \frac{AA\lambda^2}{2} - \dots) \\
 &= B + \lambda(AB - BA) + \frac{\lambda^2}{2!} (AAB - ABA - ABA + BAA) + \dots \\
 &= B + \lambda[A, B] + \frac{\lambda^2}{2!} [A, [A, B]] + \dots
 \end{aligned}$$

□

(b) We want to derive the operator identity for a time dependent operator  $A(t)$

$$\frac{d(e^A)}{dt} e^{-A} = \sum_{n=0}^{\infty} \frac{1}{(n+1)!} L_A^n \left( \frac{dA}{dt} \right) \text{ where } L_A(X) = [A, X], L_A^2(X) = [A, [A, X]], \dots$$

*Proof.* TODO

□

## PROPAGATORS AND PATH INTEGRALS

In this section we'll talk a bit about the path integral. Which is important in understanding several areas of quantum mechanics and is very useful when we go into quantum field theory and start talking about non-abelian gauge theories. We'll start our discussion with the propagator

### PROPAGATOR

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We'll start with some initial wave function  $|\psi_{t_0}\rangle$  which we want to evolve into  $|\psi_t\rangle$  with the unitary time evolution operator

$$|\psi(t)\rangle = U(t; t_0)|\psi(t_0)\rangle$$

Expanding the above in the position basis and resolving the identity gives us

$$\langle x|\psi(t)\rangle = \int dx_0 \langle x|U(t; t_0)|x_0\rangle \langle x_0|\psi(t_0)\rangle$$

We'll define the **pink term** as the propagator  $K(x, t; x_0, t_0)$ . This gives us

$$\psi(x, t) = \int dx_0 K(x, t; x_0, t_0) \psi(t_0, x_0)$$

The fact that the propagator comes from the unitary time evolution operator leads us to several useful properties

$$U(t = t_0, t_0) = 1 \Rightarrow K(x, t_0; x_0, t_0) = \langle x|x_0\rangle = \delta(x - x_0)$$

$$i\hbar\partial_t U(t, t_0) = H(t)U(t, t_0) \Rightarrow i\hbar\partial_t K = \langle x|i\hbar\partial_t U|x_0\rangle = H(t)\langle x|U|x_0\rangle = \left[-\frac{\hbar^2}{2m}\partial_x^2 + V(x, t)\right]K$$

Lets consider the simplest case of this, the 1-D free particle  $\hat{H} = \hat{p}^2/2m$ .

**EXAMPLE 3: (1-D FREE PARTICLE PROPAGATOR)** For our sanity let  $t_0 = 0$ . We then have the following form of the propagator

$$K(x, x_0; t) = \langle x|U(t)|x_0\rangle$$

$$(\text{explicit form of time evolution}) = \langle x|\exp\{-it\hat{p}^2/2m\hbar\}|x_0\rangle$$

$$(\text{resolve identity}) = \int dp \langle x|\exp\{-it\hat{p}^2/2m\hbar\}|p\rangle \langle p|x_0\rangle$$

$$(\text{act to the right with } \hat{p}) = \int dp \exp\{-itp^2/2m\hbar\} \langle x|p\rangle \langle p|x_0\rangle$$

$$(\text{use } \langle x|p\rangle \text{ from notes}) = C \int dp \exp\left\{-\frac{i}{\hbar}\left(\frac{tp^2}{2m} - p(x - x_0)\right)\right\}$$

$$(\text{gaussian integral}) = C' \exp\left\{\frac{im}{2\hbar t}(x - x_0)^2\right\}$$

Where  $C$  and  $C'$  are some constants we don't care about at the moment.

With this notion of a propagator we can go on to define path integrals

## DISCRETE AND COMPACT PATH INTEGRAL

March 14, 2021

We will now consider a general hamiltonian  $\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}(\hat{x})$ . First we'll let  $t = \epsilon N$  to divide up our unitary time evolution operator into  $N$  individual time evolutions  $\hat{U}(t) = \hat{U}(\epsilon)^N$ . This means our propagator becomes

$$K(x, x_0; t) = \langle x | U(\epsilon) \dots U(\epsilon) | x_0 \rangle$$

From here we can resolve the identity between each time evolution to get

$$K(x, x_0; t) = \int dx_1 \dots dx_{N-1} \times \langle x | U(\epsilon) | x_{N-1} \rangle \times \dots \times \langle x_1 | U(\epsilon) | x_0 \rangle$$

Now before we continue lets notice something speical about our unitary time evolution operator. If we exapnd it out we get

$$U(\epsilon) = 1 - \frac{i\epsilon}{\hbar} (\hat{T} + \hat{V}) + O(\epsilon^2)$$

And similarly we have

$$\exp\left\{-\frac{i\epsilon}{\hbar} \hat{T}\right\} \times \exp\left\{-\frac{i\epsilon}{\hbar} \hat{V}\right\} = \left(1 - \frac{i\epsilon}{\hbar} \hat{T}\right) \left(1 - \frac{i\epsilon}{\hbar} \hat{V}\right) + O(\epsilon^2) = 1 - \frac{i\epsilon}{\hbar} (\hat{T} + \hat{V}) + O(\epsilon^2)$$

So to order  $\epsilon^2$  we can write  $U(\epsilon)$  as the product of two exponentials of operators. Note that this isn't implicity true since the operators may or may not commute. Lets now consider a specific  $\langle x_{j+1} | U(\epsilon) | x_j \rangle$  with our approximation.

$$\begin{aligned} \langle x_{j+1} | U(\epsilon) | x_j \rangle &= \langle x_{j+1} | U(\epsilon) | x_j \rangle \\ (\text{use } O(\epsilon^2) \text{ approximation}) &\approx \langle x_{j+1} | \exp\left\{-\frac{i\epsilon}{\hbar} \hat{T}\right\} \times \exp\left\{-\frac{i\epsilon}{\hbar} \hat{V}\right\} | x_j \rangle \\ (\text{resolve identity}) &= \int dp \langle x_{j+1} | \exp\left\{-\frac{i\epsilon}{2m\hbar} \hat{p}^2\right\} | p \rangle \langle p | \exp\left\{-\frac{i\epsilon}{\hbar} \hat{V}(\hat{x})\right\} | x_j \rangle \\ (\text{eigenvalue equation}) &= \int dp \exp\left\{-\frac{i\epsilon}{\hbar} \left(\frac{p^2}{2m} + V(x_j)\right)\right\} \langle x_{j+1} | p \rangle \langle p | x_j \rangle \\ (\text{Oh woah we've done this before}) &= C' \exp\left\{\frac{i\epsilon}{\hbar} \left(\frac{m(x_{j+1} - x_j)^2}{2\epsilon^2} - V(x_j)\right)\right\} \end{aligned}$$

So all together we get

$$K(x, x_0; t) = (C')^{N/2} \int dx_1 \dots dx_{N-1} \times \exp\left\{\frac{i\Delta t}{\hbar} \sum_{j=0}^{N-1} \left(\frac{m\Delta x_j^2}{2\Delta t^2} - V(x_j)\right)\right\}$$

Where we've introduced  $\Delta x_j = x_{j+1} - x_j$  and  $\Delta t = \epsilon$ . The boxed result above is what we call the discrete path integral. On examination it looks like we've discretized time and are integrating

over all possible paths from  $x_0$  to  $x$ . If we (unrigorously) take the term in the exponential to the continuous limit we see that

$$\Delta t \sum_{j=0}^{N-1} \left( \frac{m \Delta x_j^2}{2 \Delta t^2} - V(x_j) \right) \rightarrow \int_0^t dt (T - V) = S[x(\tau)] = (\text{classical action})$$

Or if we go to path space  $p = \{x(\tau) | x(0) = x_0 \text{ and } x(t) = x\}$  we can write the propagator as

$$K(x, x_0; t) = (C')^{N/2} \int_p d[x(\tau)] \times \exp \left\{ \frac{i}{\hbar} S[x(\tau)] \right\}$$

This boxed result is what we call the compact path integral. However we shouldn't be too chuffed with ourselves, there was some very fast hand-waving going on above. For example, could we really take the argument of the exponential to the continuous limit? That's a questions I can't answer right now at least. Something interesting to notice. If we take  $\hbar \rightarrow 0$  we expect classical behavior to reemerge. This can be seen explicitly. As we take  $\hbar \rightarrow 0$  we find that the integrand start furiously oscillating when we integrate over path space and this causes nearby paths to cancel **unless**  $\delta S[x(\tau)] = 0$  in which case the nearby paths will be constructive. We should recognize the  $\delta S = 0$  condition from our classical mechanics class that characterizes classical paths.