Notes for Quantum Mechanics

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Updated for 2005

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Lecture 13

The commentator and anti-commutator of two operators $\hat{A}$ and $\hat{B}$ is

Commutator $[\hat{A},\hat{B}]=\hat{A}\hat{B}-\hat{B}\hat{A}$ Anti-commutator $\{\hat{A},\hat{B}\}=\hat{A}\hat{B}+\hat{B}\hat{A}$

Before going on lets make a definition

ϵ_{ijk} is the completely anti-symmetric tensor meaning e.g. ϵ_{123}=+1 ϵ_{132}=-1 (swap 2 and 3) ϵ_{312}=+1 ϵ_{321}=-1 etc and ϵ_{ijk}=0 if and 2 indices are equal

Your have shown some very important relations in your homework among the spin operators

$[\hat{S}_i, \hat{S}_j] = i\epsilon_{ijk}\hbar\hat{S}_k$ and $\{\hat{S}_i, \hat{S}_j\} = \frac{\hbar^2}{2}\delta_{ij}$

These are very important relationships. In fact the commutator relationship for spin, will be true generally for angular momentum, and is also a blueprint of the way people "quantize" theories (believe it or not - you take the classical objects - make them operators, then define a non-zero commutator that has an $\hbar$ in it. That way, in the limit of large things, the answer is classical, i.e. the commutator is zero). The anti-commutator relationship is the reason that fermions obey the pauli exclusion principle.

Lets also define $\hat{\mathbf{S}}^2=\hat{S}_x^{\,2}+\hat{S}_y^{\,2}+\hat{S}_z^{\,2}$ and we can prove that $[\hat{\mathbf{S}}^2, \hat{S}_i]=0$

First lets prove that $[\hat{A}^2, \hat{B}]=\hat{A}[\hat{A}, \hat{B}]+[\hat{A}, \hat{B}]\hat{A}$

proof $[\hat{A}^2, \hat{B}]=\hat{A}\hat{A}\hat{B}-\hat{B}\hat{A}\hat{A}=\hat{A}\hat{A}\hat{B}-\hat{B}\hat{A}\hat{A}+\hat{A}\hat{B}\hat{A}-\hat{A}\hat{B}\hat{A}=\hat{A}\hat{A}\hat{B}-\hat{B}\hat{A}\hat{A}=\hat{A}\hat{A}\hat{B}-\hat{A}\hat{B}\hat{A}+\hat{A}\hat{B}\hat{A}-\hat{B}\hat{A}\hat{A}=$

$\hat{A}(\hat{A}\hat{B}-\hat{B}\hat{A})+(\hat{A}\hat{B}-\hat{B}\hat{A})\hat{A}=\hat{A}[\hat{A}, \hat{B}]+[\hat{A}, \hat{B}]\hat{A}$

a couple things we need : $\epsilon_{kji}=-\epsilon_{ijk}$ and $\sum_{i=1}^{3}\epsilon_{ijk}\hat{S}_k\hat{S}_i=\sum_{i=1}^{3}\epsilon_{kji}\hat{S}_i\hat{S}_k$ (where we rename i⟷k) so then

$[\hat{\mathbf{S}}^2, \hat{S}_j]=\sum_{i=1}^{3}[\hat{S}_i^{\,2}, \hat{S}_j]=\sum_{i=1}^{3}\hat{S}_i[\hat{S}_i, \hat{S}_j]+[\hat{S}_i, \hat{S}_j]\hat{S}_i=i\hbar(\sum_{i=1}^{3}\epsilon_{ijk}\hat{S}_i\hat{S}_k+\sum_{i=1}^{3}\epsilon_{ijk}\hat{S}_k\hat{S}_i)=$

$=i\hbar(\sum_{i=1}^{3}\epsilon_{ijk}\hat{S}_i\hat{S}_k+\sum_{i=1}^{3}\epsilon_{kji}\hat{S}_i\hat{S}_k)=i\hbar(\sum_{i=1}^{3}\epsilon_{ijk}\hat{S}_i\hat{S}_k-\sum_{i=1}^{3}\epsilon_{ijk}\hat{S}_i\hat{S}_k)=i\hbar\sum_{i=1}^{3}\epsilon_{ijk}(\hat{S}_i\hat{S}_k-\hat{S}_i\hat{S}_k)=0$

Now $\{\hat{S}_i, \hat{S}_j\} = \frac{\hbar^2}{2}\delta_{ij}$ means $\hat{S}_i^{\,2}=\frac{\hbar^2}{4}$ and $\hat{\mathbf{S}}^2=\frac{3\hbar^2}{4}$

Degeneracy (two eigenkets with the same eigenvalue)

Lets go over what we mean by a basis. We start with an observable $\hat{A}$ with eigenkets $|a_i\rangle$ and eigenvalues a_i and the index i runs from i=1,n where n is the total number of eigenkets. We proved that the eigenkets $|a_i\rangle$ formed an orthogonal set which spans the space assuming that no two of the eigenkets a_i were the same. It turns out in some very important cases, that there are eigenkets with the same eigenvalues, i.e. where $a_i = a_j$ for some i and j. Such eigenkets are said to be degenerate. For instance suppose the operator $\hat{A}$ is a Hamiltonian (the energy operator) and we have two states $\hat{B}$ with the same energy - e.g. the two electrons in the 1p state of hydrogen (if you remember this). In any case there are two lowest energy states which have the same energy in hydrogen. Fortunately in practical applications, there is usually another observable which comminutes with $\hat{A}$ which can be used to label the degenerate eigenkets. In the case of hydrogen, there is one electron which has a $\frac{+1}{2}$ spin and the other has a $\frac{-1}{2}$ spin. So in this case we have two observably which are used to label the eigenkets - this means that the eigenkets must be simultaneously eigenkets of both $\hat{A}$ and $\hat{B}$ and we can label the kets $|a_i, b_i\rangle$ So we had better study such pairs of observables.

Compatible Observables

Two observables $\hat{A}$ and $\hat{B}$ are said to be compatible if $[\hat{A}, \hat{B}]=0$ and incompatible if $[\hat{A}, \hat{B}]\neq 0$ (5)

Theorem : Suppose that $\hat{A}$ and $\hat{B}$ are compatible observables (i.e. $[\hat{A}, \hat{B}] = 0$) and the eigenvalues of $\hat{A}$ are non – degenerate. Then the matrix elements $\langle a_i | \hat{B} | a_j \rangle$ are all diagonal. (Recall that the matrix elements of $\hat{A}$ are already diagonal if $| a_i \rangle$ are used as eigenkets) (6)

Proof : $\langle a_i | [\hat{A}, \hat{B}] | a_j \rangle = \langle a_i | \hat{A}\hat{B} - \hat{B}\hat{A} | a_j \rangle = (a_i - a_j) \langle a_i | \hat{B} | a_j \rangle = 0$ so $\langle a_i | \hat{B} | a_j \rangle = 0$ unless $a_i = a_j$ QED

So we can write $\langle a_i | \hat{B} | a_j \rangle = \langle a_i | \hat{B} | a_i \rangle \delta_{ij}$ Then we can write $\hat{B}$ as

$$\hat{B} = \hat{1}\hat{B}\hat{1} = \sum_{i,j} | a_i \rangle \langle a_i | \hat{B} | a_j \rangle \langle a_j | = \sum_{i,j} | a_i \rangle \langle a_i | \hat{B} | a_i \rangle \delta_{ij} \langle a_j | = \sum_i | a_i \rangle \langle a_i | \hat{B} | a_i \rangle \langle a_i |$$

Now lets find out what happens if we operate on an eigenket $| a_j \rangle$

$$\hat{B} | a_j \rangle = \sum_i | a_i \rangle \langle a_i | \hat{B} | a_i \rangle \langle a_i | a_j \rangle = \sum_i | a_i \rangle \langle a_i | \hat{B} | a_i \rangle \delta_{ij} = \langle a_j | \hat{B} | a_j \rangle | a_j \rangle$$

So $| a_j \rangle$ is an eigenket of $\hat{B}$ with eigenvalue $\langle a_j | \hat{B} | a_j \rangle$ which we will call b_j (7)

So we will label the ket now as $|a_i, b_i\rangle$ since it is a simultaneous eigenket of both $\hat{A}$ and $\hat{B}$ and we have

$$\hat{A} |a_i, b_i\rangle = a_i | a_i, b_i \rangle \text{ and } \hat{B} |a_i, b_i\rangle = b_i | a_i, b_i \rangle$$

(As a notational thing sometimes we will use a collective index k_i to stand for the set a_i, b_i i.e. $| k_i \rangle = | a_i, b_i \rangle$) (8)

Now suppose that the operator $\hat{A}$ has a degeneracy, that is $a_i = a_j$ for a particular i and j. This means we may have $\langle a_i | \hat{B} | a_j \rangle \neq 0$ where $i \neq j$, meaning that $\hat{B}$ is not diagonal for this pair.

To fix this we can construct the appropriate linear combinations of $|a_i\rangle$ and $|a_j\rangle$ which diagonalizes $\hat{B}$ using the diagonalization procedure that we learned before.

We can generalize this to several commuting (i.e. compatible) observables so $[\hat{A}, \hat{B}] = [\hat{B}, \hat{C}] = [\hat{A}, \hat{C}] = ... = 0$

We can assume we have found a maximal set of commuting observables $\hat{A}, \hat{B}, \hat{C}$, ... so we cannot find any more which commute. Each of the operators may have degeneracies but we will assume that if we specify all the eigenvalues a,b,c,... then the eigenket $|a, b, c, ...\rangle$ is uniquely specified. So now we can write $|k_i\rangle = |a_i, b_i, c_i, ...\rangle$ and $\langle k_i | k_j\rangle = \delta_{ij}$ and $\sum_i |k_i\rangle\langle k_i| = 1$

Ok now lets see what happens when we make measurements. $\hat{A}$ and $\hat{B}$ are compatible. We make a measurement of $\hat{A}$ which puts the ket into an eigenket of $\hat{A}$ (which is also an eigenket of $\hat{B}$) We can then make a measurement of $\hat{B}$ and get the result b. If we make a measurement of $\hat{A}$ it give us the eigenvalue a as before. So things make sense.

$$|\alpha\rangle \xrightarrow{A\text{ meaurement}} |a, b\rangle \xrightarrow{B\text{ meassurement}} |a, b\rangle \xrightarrow{A\text{ measurement}} |a, b\rangle$$

Now when there is a degeneracy in $\hat{A}$ (i.e. $a_i = a_j$) then the measurement yields a measurement $a_i = a_j$ so we don't know if the eigenket is $|a_i\rangle$ or $|a_j\rangle$. They can be differentiated only by the eigenvalues of $\hat{B}$. Lets just call $a = a_i = a_j$ It ends up being a linear combination of the two. Then a measurement of $\hat{B}$ will choose one of the eigenvalues. So it goes like this

$$|\alpha\rangle \xrightarrow{A\text{ meaurement}} c_i\,|a, b_i\rangle + c_j\,|a, b_j\rangle \xrightarrow{B\text{ meassurement}} |a, b_i\rangle \xrightarrow{A\text{ measurement}} |a, b_i\rangle$$

Here the c's must be appropriately normalized $\sqrt{c_i^2 + c_j^2} = 1$

So compatible observables can be measured one after the other without messing the other measurement up, and can also be used to resolve degeneracies.

Incompatible Observables

Now we turn to incompatible observables, which lies at the heart of quantum mechanics, and will lead to the Hessenberg Uncertainty relationship. Compatible observables had a complete set of simultaneous eigenkets. We will want to prove that Incompatible observables do NOT have a complete set of simultaneous eigenkets. Let us assume that the converse is true and we will come to a contradiction. (9)

Proof by contradiction

$[\hat{A}, \hat{B}] \neq 0$; We will label the complete set of simultaneous eigenkets as $|a_i, b_i\rangle$

$\hat{A}\,\hat{B}\,|a_i, b_i\rangle = \hat{A}\,b_i\,|a_i, b_i\rangle = b_i\,\hat{A}\,|a_i, b_i\rangle = b_i\,a_i|a_i, b_i\rangle = a_i\,b_i|a_i, b_i\rangle$

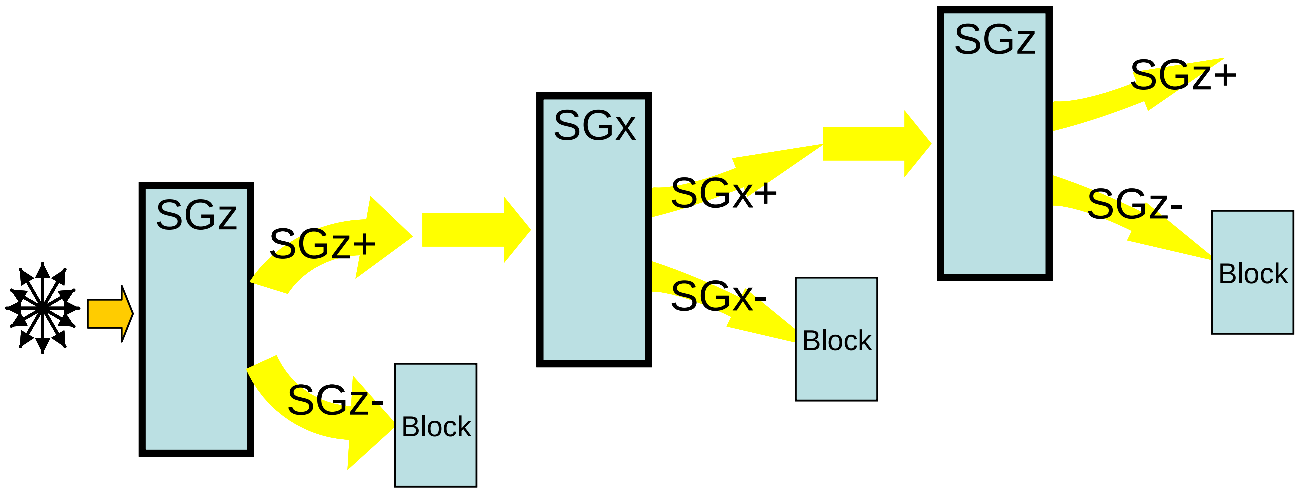
$\hat{B}\hat{A}\,|a_i, b_i\rangle = \hat{B}\,a_i\,|a_i, b_i\rangle = a_i\,\hat{B}\,|a_i, b_i\rangle = a_i\,b_i|a_i, b_i\rangle$ Now subtract the two and we get

$[\hat{A}, \hat{B}] = 0$ which is a contradiction QED

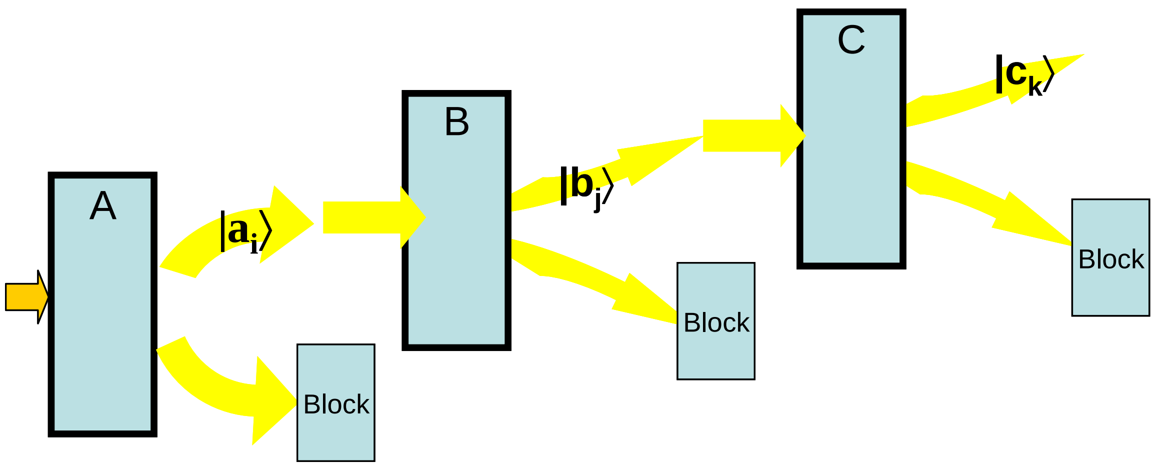
Back to the Stern-Gerlach Experiment

Let us think back now to the SG experiment where we have now measured SGz in the last apparatus.

we know $[S_z, S_x] \neq 0$ that is, they are not compatible.



Now lets make it more general and call them just $\hat{A}$, $\hat{B}$, $\hat{C}$

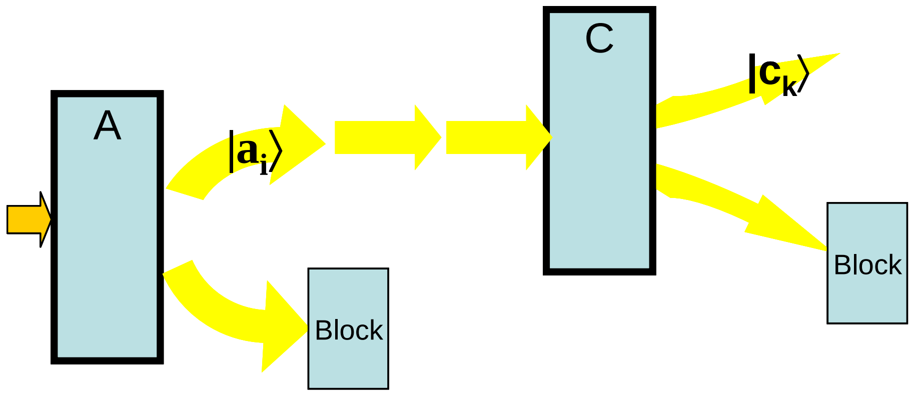


$$P = |\langle b_j|a_i\rangle|^2 \qquad P = |\langle c_k|b_j\rangle|^2 |\langle b_j|a_i\rangle|^2$$

Now lets see if we can follow the a state through. We will start with the ket $|a_i\rangle$ as it enters into the $\hat{B}$ apparatus

So we start with $|a_i\rangle$. Now we make a measurement of $\hat{B}$. What is the probability that we will make a measurement b_j and that the ket coming out will be $|b_j\rangle$? Its $P = |\langle b_j|a_i\rangle|^2$. What is the probability then that C will make a measurement c_k? We have to multiply the probabilities together to get $P = |\langle c_k|b_j\rangle|^2 \, |\langle b_j|a_i\rangle|^2$. Now lets look at this. It tells us what the probability that $|a_i\rangle$ finally comes out $|c_k\rangle$. But we have chosen an intermediary which is $|b_j\rangle$. So let sum over all the b_j's to get the total probability that $|a_i\rangle$ finally comes out $|c_k\rangle$.
$P = \sum_j |\langle c_k|b_j\rangle|^2 \, |\langle b_j|a_i\rangle|^2 = \sum_j \langle c_k|b_j\rangle\langle b_j|a_i\rangle\langle a_i|b_j\rangle\langle b_j|c_k\rangle$. Note this is the probability that we get $|c_k\rangle$ from $|a_i\rangle$ going though ANY $|b_j\rangle$

Now lets try another arrangement



$P = \,|\langle c_k|a_i\rangle|^2 = |\langle c_k|\hat{1}|a_i\rangle|^2 = |\langle c_k|\sum_j|b_j\rangle\langle b_j|a_i\rangle|^2 = |\sum_j\langle c_k|b_j\rangle\langle b_j|a_i\rangle|^2 = \sum_j\langle c_k|b_j\rangle\langle b_j|a_i\rangle\sum_l\langle a_i|b_l\rangle\langle b_l|c_k\rangle =$
$\sum_j\sum_l\langle c_k|b_j\rangle\langle b_j|a_i\rangle\langle a_i|b_l\rangle\langle b_l|c_k\rangle$

A DIFFERENT ANSWER than we got above!! i.e. $\sum_j\sum_l\langle c_k|b_j\rangle\langle b_j|a_i\rangle\langle a_i|b_l\rangle\langle b_l|c_k\rangle \neq \sum_j\langle c_k|b_j\rangle\langle b_j|a_i\rangle\langle a_i|b_j\rangle\langle b_j|c_k\rangle$.

The extra terms are $\sum_{\mathrm{jl},\,j\neq l}\langle c_k|b_j\rangle\langle b_j|a_i\rangle\langle a_i|b_l\rangle\langle b_l|c_k\rangle$. Its sort of all the pieces which, in the middle are NOT an eigenket of $\hat{B}$ but are a mixture of eigenkets of $\hat{B}$

Now if $[\hat{A},\hat{B}] = 0$ or $[\hat{B},\hat{C}] = 0$ then the two probabilities become equal.

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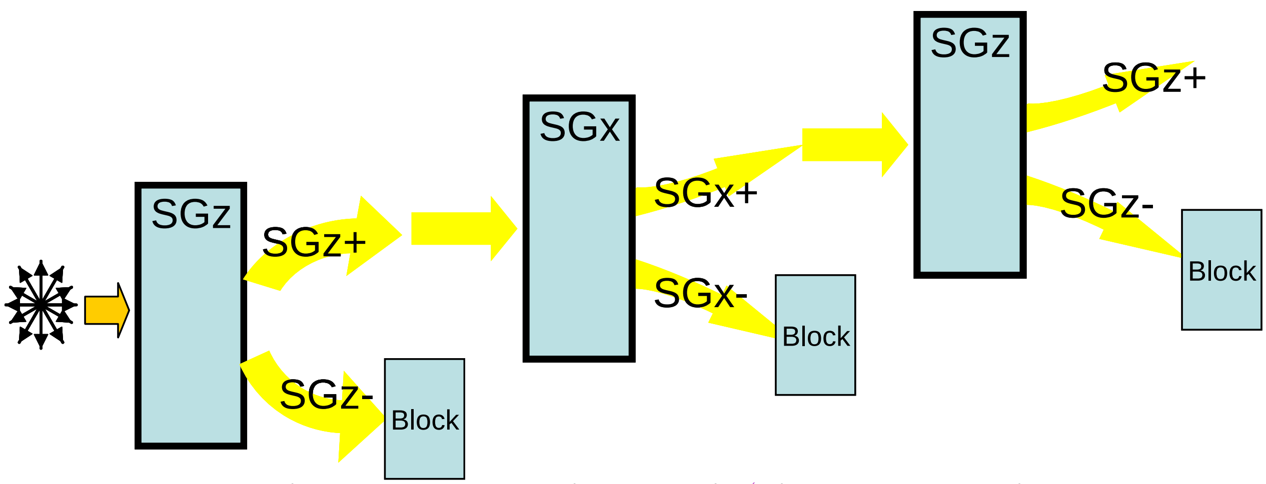

$|+\rangle = \frac{1}{\sqrt{2}}(|S_x+\rangle + |S_x-\rangle)$ $\quad \frac{1}{\sqrt{2}}|S_x+\rangle = \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)\right)$ $\quad \frac{1}{2}|+\rangle$

Lets now think about this in terms of the SG experiment. Lets let $\hat{A}$=SGz, $\hat{B}$=SGx, $\hat{C}$=SGz,

We will take the first situation where we use all three. We start with an $|a_i\rangle$=|SGz;+⟩ beam. It then goes through SGx. We can write |SGz;+⟩ = $\frac{1}{\sqrt{2}}$(|SGx;+⟩ +|SGx;-⟩). After going through the SGx apparatus it will either be |SGx;+⟩ or |SGx;-⟩ . Lets not renomalize so we can compare to the initial |SGz;+⟩ intensity. So we will write the state after SGx as either $\frac{1}{\sqrt{2}}$|SGx;+⟩ or $\frac{1}{\sqrt{2}}$(|SGx;-⟩.

Remembering |SGx; +⟩=$\frac{1}{\sqrt{2}}$(|+⟩+|−⟩) and |SGx; −⟩=$\frac{1}{\sqrt{2}}$(|+⟩-|−⟩) the state after SGx ($\hat{B}$) not renomalized is either

$|b_j\rangle = \frac{1}{\sqrt{2}}|\text{SGx}; +\rangle = \frac{1}{2}(|+\rangle + |-\rangle)$ or $|b_j\rangle = \frac{1}{\sqrt{2}}|\text{SGx}; -\rangle = \frac{1}{2}(|+\rangle - |-\rangle)$

Now lets assume that we got an $|\text{SGx}; +\rangle$ after measurement i.e. $|b_j\rangle = \frac{1}{\sqrt{2}}|\text{SGx}; +\rangle = \frac{1}{2}(|+\rangle + |-\rangle)$

Now after we go through the SGz apparatus ($\hat{C}$) lets assume we get $|+\rangle$, so the final state is $|c_k\rangle = \frac{1}{2}|+\rangle$ the magnitude of this is $= \frac{1}{4}$

Now after going through SGx ($\hat{B}$) we could have gotten an $|\text{SGx};-\rangle$ and this would give us another $\frac{1}{4}$. So the total chance of getting a $|+\rangle$ at the end is $\frac{1}{2}$.

Lets now take the second case. We start with a $|\text{SGz};+\rangle$ beam. Now there is no SGx apparatus. It goes directly into the SGz ($\hat{C}$) apparatus so starting with a $|+\rangle$ beam, the chances of measuring a $|+\rangle$ beam after ($\hat{C}$) is 1 !!!. A different answer.

So it makes a difference whether or no we measure $\hat{B}$ or not even though we still let everything through! What does the measurement of $\hat{B}$ do? It forces the beam in the middle to be in and eigenstate of SGx, i.e. $|\text{SGx};+\rangle$ or $|\text{SGx};-\rangle$. If we don't make the measurement then the intermediate state could be a mixture of the two. So the measurement actually limits the possibilities. Such is the strangeness of Quantum mechanics.

Note: Rememnber I had told you before the last lecture that I was confused about an example. I had picked a case where $\hat{C}$ was a measurement of Sy. This is a case where the cross terms cancel and the two cases give the same answer! This was a special case and is not true in general as you can see by the example I picked above. I found the problem by writing out all terms (16) and watching the cross terms cancel. It was worth it.

