Notes for Quantum Mechanics

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Lecture 12

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Lecture 12

Changing basis (or "representation")

We have decided to use the S_z basis, i.e. $|+\rangle$ and $|-\rangle$. Suppose we want to switch to the S_x basis. Is the a way to do this? Before we answer this, lets see if there is a way to go from one set of eigenkets say $|+\rangle$ and $|-\rangle$, to another set, perhaps $|S_x+\rangle$ and $|S_x-\rangle$. Lets think of this more generally as $\hat{A}=\hat{S}_z$ with eigenkets $|a_i\rangle$. Is there a way to find a different set of eigenkets of another operator $\hat{B}=\hat{S}_x$ with eigenkets $|b_i\rangle$? In general we can let $\hat{A}$ and $\hat{B}$ be any two operators which represent observables so that the kets $|a_i\rangle$ and $|b_i\rangle$are complete, orthogonal eigenkets. Let us suppose that we have an operator $\hat{U}$ which does this.

i.e. $|b_i\rangle=\hat{U}|a_i\rangle$. (1)

The operator $\hat{U}$ will be a special kind of transformation matrix called a unitary operator.

A unitary operator $\hat{U}$ is one in which $\hat{U}^\dagger \hat{U}=\hat{1}$ and $\hat{U}\hat{U}^\dagger=\hat{1}$ This also means $\hat{U}^{-1}=\hat{U}^\dagger$ (2)

Now we want an operator $\hat{U}$ such that $|b_i\rangle=\hat{U}|a_i\rangle$. By construction this will be $\sum_k |b_k\rangle\langle a_k|$ (3)

Proof: $\hat{U}|a_i\rangle = \sum_k |b_k\rangle\langle a_k | a_i\rangle = \sum_k |b_k\rangle\,\delta_{\mathrm{ki}}=|b_i\rangle$ QED

we can also show that this is unitary: $\hat{U}^\dagger \hat{U}=\sum_j |a_j\rangle\langle b_j|\sum_k |b_k\rangle\langle a_k| =\sum_j \sum_k |a_j\rangle\langle b_j|b_k\rangle\langle a_k| =\sum_j |a_j\rangle\langle a_j| =\hat{1}$

Now we can think of $\hat{U}$ in a matrix notation. The matrix elements are (see lecture 7)

$\langle a_i|\hat{U}|a_j\rangle= \langle a_i|\sum_k |b_k\rangle\langle a_k|a_j\rangle= \langle a_i|b_j\rangle$ so for the a two component case $\hat{U}=\begin{pmatrix} \langle a_1|b_1\rangle & \langle a_1|b_2\rangle \\ \langle a_2|b_1\rangle & \langle a_2|b_2\rangle \end{pmatrix}$ (4)

where we have used (3). Now lets see how we can use this.

We have typically written things in the S_z basis, but suppose we want to switch to a different basis, say S_x. How do we do this?

First lets start out by figuring out how to change the basis of kets. In the S_z basis we write $|\alpha\rangle=|+\rangle\langle+|\alpha\rangle+|-\rangle\langle-|\alpha\rangle$.

So that we can write this symbolically as $|\alpha\rangle=\sum_i |a_i\rangle\, c_i = \sum_i |a_i\rangle\langle a_i|\alpha\rangle$ where the $|a_i\rangle$ are eigenkets of $\hat{A}$ and $\hat{A}=\hat{S}_z$. We see that the coefficients $c_i = \langle a_i|\alpha\rangle$. Now lets let $\hat{B}=\hat{S}_x$ and $|b_i\rangle$ are the eigenkets. In general we can let $\hat{A}$ and $\hat{B}$ be any two operators which represent observables so that the kets $|a_i\rangle$ and $|b_i\rangle$are complete, orthogonal eigenkets. Remember $\sum_i |a_i\rangle\langle a_i| = \hat{1}$ and $\sum_i |b_i\rangle\langle b_i|=\hat{1}$ Then we can write

$|\alpha\rangle=\sum_i |a_i\rangle\langle a_i|\alpha\rangle=\sum_{ij} |b_j\rangle\langle b_j|a_i\rangle\langle a_i|\alpha\rangle=\sum_j |b_j\rangle\sum_i\langle b_j|a_i\rangle\langle a_i|\alpha\rangle$ So we can now write $|\alpha\rangle=\sum_j |b_j\rangle\, c'_j$ where the new coefficients $\langle b_j|\alpha\rangle=c'_j=\sum_i\langle b_j|a_i\rangle\langle a_i|\alpha\rangle$. Thinking of this in matrix notation is particularly nice since originally in the $\hat{A}$ basis we write a column vector $\begin{pmatrix}\langle a_1|\alpha\rangle\\ \langle a_2|\alpha\rangle\end{pmatrix}$

We can transform to the new basis as follows: $\begin{pmatrix}\langle b_1|\alpha\rangle\\ \langle b_2|\alpha\rangle\end{pmatrix}=\begin{pmatrix}\langle b_1|a_1\rangle & \langle b_1|a_2\rangle\\ \langle b_2|a_1\rangle & \langle b_2|a_2\rangle\end{pmatrix}\begin{pmatrix}\langle a_1|\alpha\rangle\\ \langle a_2|\alpha\rangle\end{pmatrix}$. (5)

Notice how this matrix multiplication does exactly the same thing as the sum. Now notice that this matrix is just the transpose-complex conjugate of $\hat{U}$ so we can write

$\begin{pmatrix}\langle b_1|\alpha\rangle\\ \langle b_2|\alpha\rangle\end{pmatrix}=\hat{U}^\dagger\begin{pmatrix}\langle a_1|\alpha\rangle\\ \langle a_2|\alpha\rangle\end{pmatrix}$ where it is now understood that $\hat{U}$ is in matrix notation. i.e. (6)

(new basis)=$\hat{U}^\dagger$(old basis) (7)

Example:

Lets first recall from Lecture 8:

$|S_x;\pm\rangle=\frac{1}{\sqrt{2}}(|+\rangle\pm|-\rangle)$ $\quad |S_y;\pm\rangle=\frac{1}{\sqrt{2}}(|+\rangle\pm i|-\rangle)$ (a)

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

$|+\rangle=\frac{1}{\sqrt{2}}(|S_y+\rangle+|S_y-\rangle)$ $\quad |-\rangle=\frac{1}{\sqrt{2}\,i}(|S_y+\rangle-|S_y-\rangle)$ (c)

Now lets take $|\pm\rangle$ as the old basis and $|S_x\pm\rangle$ as the the new basis

1) find the representation of $|\pm\rangle$ in the $|S_x\pm\rangle$ basis. We know what the answer should be just by looking at (b). It should be $|+\rangle=\frac{1}{\sqrt{2}}(|S_x+\rangle+|S_x-\rangle)\doteq\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$ and $|-\rangle=\frac{1}{\sqrt{2}}(|S_x+\rangle-|S_x-\rangle)\doteq\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$ in the $|S_x\pm\rangle$ basis. Its very important that we recall we are in the $|S_x\pm\rangle$ basis! Lets now use what we learned to see if we get the same answer.

$\hat{U}\doteq\begin{pmatrix}\langle \text{old}_1|\text{new}_1\rangle & \langle \text{old}_1|\text{new}_2\rangle\\ \langle \text{old}_2|\text{new}_1\rangle & \langle \text{old}_2|\text{new}_2\rangle\end{pmatrix}=\begin{pmatrix}\langle+|S_x+\rangle & \langle+|S_x-\rangle\\ \langle-|S_x+\rangle & \langle-|S_x-\rangle\end{pmatrix}==\frac{1}{\sqrt{2}}\begin{pmatrix}\langle+|(|+\rangle+|-\rangle) & \langle+|(|+\rangle-|-\rangle)\\ \langle-|(|+\rangle+|-\rangle) & \langle-|(|+\rangle-|-\rangle)\end{pmatrix}=\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\1 & -1\end{pmatrix}$

$\hat{U}^\dagger=\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\1 & -1\end{pmatrix}$ so using (7) we can write $|\pm\rangle$ which in the original basis is just $\begin{pmatrix}1\\0\end{pmatrix}$ and $\begin{pmatrix}0\\1\end{pmatrix}$

$|+\rangle\doteq\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\1 & -1\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix}=\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$ $\quad |-\rangle\doteq\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\1 & -1\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix}=\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$ in the new basis as we expected.

How does this change the matrix elements of operators? Lets find out for an operator $\hat{X}$, Remembering that $|b_i\rangle=\hat{U}|a_i\rangle$ and hence $\langle b_i|=\langle a_i|\hat{U}^\dagger$

$\langle b_k \mid \hat{X} \mid b_l\rangle = \langle b_k \mid \hat{1}\,\hat{X}\,\hat{1} \mid b_l\rangle = \langle b_k \mid \sum_i |a_i\rangle\langle a_i| \hat{X} \mid \sum_j |a_j\rangle\langle a_j| b_l\rangle = \sum_i\sum_j \langle a_k|\hat{U}^\dagger|a_i\rangle\langle a_i|\hat{X} \mid \sum_j |a_j\rangle\langle a_j|\hat{U}|a_l\rangle =$
$= \langle a_k|\hat{U}^\dagger\hat{X}\hat{U}|a_l\rangle$ or in somewhat symbolic notation where we mean that $\hat{X}'$ is just the matrix for $\hat{X}$ in a new basis or representation

$\hat{X}' = \hat{U}^\dagger\hat{X}\hat{U}$ - This is known as a similarity transformation in matrix algebra.

So to summarize (ket in new basis)$=\hat{U}^\dagger$(ket old basis) AND $\hat{X}' = \hat{U}^\dagger\hat{X}\hat{U}$ (8)

Example:

2) Now $\hat{S}_x$ in the $|\pm\rangle$ basis is $\frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$. Lets write it in the $|S_x;\pm\rangle$ basis. We again know what the answer has to be - it has to be $\frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$. Lets use our methods and see if that is what we get. We use (8)

$\hat{U}^\dagger\hat{S}_x\hat{U} = \frac{\hbar}{2}\frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix} = \frac{\hbar}{2}\frac{1}{2}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}1 & -1\\ 1 & 1\end{pmatrix} = \frac{\hbar}{2}\frac{1}{2}\begin{pmatrix}2 & 0\\ 0 & -2\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$ as we expected.

TRACE

Now we define a trace of an operator as the sum of the diagonal elements

$\mathrm{Tr}(\hat{X}) = \sum_i \langle a_i \mid \hat{X} \mid a_i\rangle$. This turns out to be INDEPENDENT of representation (9)

Proof: $\sum_i \langle a_i \mid \hat{X} \mid a_i\rangle = \sum_i \langle a_i \mid \sum_k |b_k\rangle\langle b_k|\hat{X} \mid \sum_l |b_l\rangle\langle b_l|a_i\rangle = \sum_k\sum_l\sum_i \langle a_i \mid b_k\rangle\langle b_k|\hat{X} \mid |b_l\rangle\langle b_l|a_i\rangle =$
$= \sum_k\sum_l\sum_i \langle b_l|a_i\rangle\langle a_i \mid b_k\rangle\langle b_k|\hat{X} \mid b_l\rangle = \sum_k\sum_l \langle b_l|\hat{1} \mid b_k\rangle\langle b_k|\hat{X} \mid b_l\rangle = \sum_k\sum_l \delta_{kl}\langle b_k|\hat{X} \mid b_l\rangle = \sum_k\langle b_k|\hat{X} \mid b_k\rangle$ QED

A few other things I will ask you to prove in the problem set

$\mathrm{Tr}(\hat{X}\hat{Y}) = \mathrm{Tr}(\hat{Y}\hat{X})$
$\mathrm{Tr}(\hat{U}^\dagger\hat{X}\hat{U}) = \mathrm{Tr}(\hat{X})$
$\mathrm{Tr}(|a_i\rangle\langle a_j|) = \delta_{ij}$
$\mathrm{Tr}(|b_i\rangle\langle a_i|) = \langle a_i|b_i\rangle$ (10)

Example:

3) Now in example 2 we had two representation of $\hat{S}_x$ as $\frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$ in the usual $|\pm\rangle$ and as $\frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$ in the $|S_x;\pm\rangle$. The trace is the same (i.e. zero) in either basis.

Example:

4) now lets try something harder. Let's write $|S_x;\pm\rangle$ in the $|S_y;\pm\rangle$ basis. So we have

$|\pm\rangle$ old basis and $|S_y\pm\rangle$ new basis

$$\hat{U} \doteq \begin{pmatrix} \langle \text{old}_1 | \text{new}_1\rangle & \langle \text{old}_1 | \text{new}_2\rangle \\ \langle \text{old}_2 | \text{new}_1\rangle & \langle \text{old}_2 | \text{new}_2\rangle \end{pmatrix} = \begin{pmatrix} \langle + | S_y +\rangle & \langle + | S_y -\rangle \\ \langle - | S_y +\rangle & \langle - | S_y -\rangle \end{pmatrix} ==$$

$$\frac{1}{\sqrt{2}} \begin{pmatrix} \langle + |(|+\rangle + i\,|-\rangle) & \langle + |(|+\rangle - i\,|-\rangle) \\ \langle - |(|+\rangle + i\,|-\rangle) & \langle - |(|+\rangle - i\,|-\rangle) \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}$$

$$\hat{U}^\dagger = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}$$

In the original $|\pm\rangle$ basis $|S_x+\rangle \doteq \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$ and $|S_x-\rangle \doteq \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$

In the new basis $|S_x+\rangle \doteq \frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}}\begin{pmatrix}1 & -i\\1 & i\end{pmatrix}\begin{pmatrix}1\\1\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1-i\\1+i\end{pmatrix}$ $|-\rangle \doteq \frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}}\begin{pmatrix}1 & -i\\1 & i\end{pmatrix}\begin{pmatrix}1\\-1\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1+i\\1-i\end{pmatrix}$

What does this mean? It means

$|S_x+\rangle = \frac{1}{2}(1\text{-i})\,|S_y+\rangle + \frac{1}{2}(1\text{+i})\,|S_y-\rangle$ and $|S_x-\rangle = \frac{1}{2}(1\text{+i})\,|S_y+\rangle + \frac{1}{2}(1\text{-i})\,|S_y-\rangle$

Lets plug in for $|S_y\pm\rangle$ and see if it makes sense

$|S_x+\rangle = \frac{1}{2}\frac{1}{\sqrt{2}}(1\text{-i})(|+\rangle + \text{i}|-\rangle) + \frac{1}{2}\frac{1}{\sqrt{2}}(1\text{+i})(|+\rangle - \text{i}|-\rangle) = \frac{1}{2}\frac{1}{\sqrt{2}}(|+\rangle + \text{i}|-\rangle - \text{i}|+\rangle + |-\rangle + \ |+\rangle - \text{i}|-\rangle + \text{i}|+\rangle + |-\rangle) = \frac{1}{2}\frac{1}{\sqrt{2}}(2|+\rangle + 2|-\rangle)$

$= \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)$ So it checks out. You can do the same for $|S_x-\rangle$

2) Now $\hat{S}_x$ in the $|\pm\rangle$ basis is $\frac{\hbar}{2}\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}$. Lets write it in the $|S_y;\pm\rangle$ basis.

$$\hat{U}^\dagger\,\hat{S}_x\,\hat{U} = \frac{\hbar}{2}\frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}}\begin{pmatrix}1 & -i\\1 & i\end{pmatrix}\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}\begin{pmatrix}1 & 1\\i & -i\end{pmatrix} = \frac{\hbar}{2}\frac{1}{2}\begin{pmatrix}1 & -i\\1 & i\end{pmatrix}\begin{pmatrix}i & -i\\1 & 1\end{pmatrix} = \frac{\hbar}{2}\frac{1}{2}\begin{pmatrix}0 & -2i\\2i & 0\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}0 & -i\\i & 0\end{pmatrix}$$ is

the representation of $\hat{S}_x$ in the $|\hat{S}_y\pm\rangle$ basis.

Diagonalization:

Suppose we know the matrix elements $\langle a_i|\hat{B}|a_j\rangle$ where the $|a_j\rangle$ are not the eigenkets of $\hat{B}$. How do we find the basis in which a matrix is diagonal? i.e. we want to find $\hat{B}$ in the $|b_j\rangle$ basis. OK - so let's first lets look at an operator $\hat{B}$ in the basis of its eigenkets $|b_j\rangle$ where $\hat{B}\,|b_j\rangle = b_j|b_j\rangle$. Now do the following

$\langle b_i\,|\,\hat{B}\,|\,b_j\rangle = b_j\langle b_i\,|\,b_j\rangle = \ b_j\,\delta_{\text{ij}}$ So in this basis $\hat{B}$ is diagonal. If we find the unitary operator where

$|b_i\rangle = \hat{U}\,|a_i\rangle$ then we know that $\hat{U}^\dagger\hat{B}\hat{U}$ is diagonal. So we have to find $\hat{U}$ such that $|b_i\rangle = \hat{U}\,|a_i\rangle$ and the $|b_i\rangle$ are eigenvectors of $\hat{B}$.

So first we want to find the eigenvectors and eigenvalues of an operator $\hat{B}$ where we know the matrix elements $\langle a_i|\hat{B}|a_j\rangle$ and where the $|a_j\rangle$ are not the eigenkets of $\hat{B}$. This means we want to find the b_j's such that

$\hat{B}\,|b_j\rangle = b_j|b_j\rangle$ where the $|b_j\rangle$'s are eigenkents of $\hat{B}$

First lets do some things to this:

$$\langle a_i\,|\,\hat{B}\,|\,b_j\rangle = b_j\langle a_i\,|\,b_j\rangle \implies \langle a_i\,|\,\hat{B}\,\hat{1}\,|\,b_j\rangle = b_j\,\langle a_i\,|\,b_j\rangle \implies \sum_k \langle a_i\,|\,\hat{B}\,|\,a_k\rangle\langle a_k\,|\,b_j\rangle = b_j\langle a_i\,|\,b_j\rangle$$

writing this in matrix notation for a 2x2 for example we have two eqn, one for each eigenvalue $b_j = b_1$ and b_2

$$\begin{pmatrix} \langle a_1 \mid \hat{B} \mid a_1 \rangle & \langle a_1 \mid \hat{B} \mid a_2 \rangle \\ \langle a_2 \mid \hat{B} \mid a_1 \rangle & \langle a_2 \mid \hat{B} \mid a_2 \rangle \end{pmatrix} \begin{pmatrix} \langle a_1 \mid b_j \rangle \\ \langle a_2 \mid b_j \rangle \end{pmatrix} = b_j \begin{pmatrix} \langle a_1 \mid b_j \rangle \\ \langle a_2 \mid b_j \rangle \end{pmatrix}$$

then from knowing a bit of linear algebra we can solve this as

$\det(\hat{B}\text{-}\lambda\hat{1})= 0$ where the values of λ will be the eigenvalues b_j. Once we solve for the b_j we can find the eigenvectors $|b_j\rangle$ which in matrix notation is $\begin{pmatrix} \langle a_1 \mid b_j \rangle \\ \langle a_2 \mid b_j \rangle \end{pmatrix}$. Now define $x_{ij} = \langle a_i \mid b_j \rangle$. But from (4) x_{ij} is just the expression for the unitary operator we want since $\langle a_i |\hat{U}|a_j\rangle = \langle a_i |b_j\rangle$. So all we have to do is to put the eigenvectors $|b_j\rangle$ in the $|a_i\rangle$ basis, side by side and we get $\hat{U}$. Note that for this procedure to work it is important that $\hat{B}$ be hermitian. e.g. $\hat{S}_+$ in the S_z basis is $\hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ and the procedure will fail since $(\hat{B}\text{-}\lambda\hat{1})\begin{pmatrix} \langle a_1 \mid b_j \rangle \\ \langle a_2 \mid b_j \rangle \end{pmatrix}= 0$ just give 0=0. (This is since one of the eigenkets is $\begin{pmatrix} 0 \\ 0 \end{pmatrix}$).

So to summarize: To diagonalize an operator
1) Find the eigenvalues b_i and eigenvectors $|b_i\rangle$ in the original basis $|a_i\rangle$
2) form $\hat{U}$ where $\langle a_i |\hat{U}|a_j\rangle = \langle a_i |b_j\rangle$ (11)
3) then diagonalize as $\hat{B}' = \hat{U}^\dagger \hat{B} \hat{U}$ where $\hat{B}'$ is now diagonal

Example:

5) now lets start with $\hat{S}_x$ in the S_z representation and change it to the S_x representation where it should be diagonal.

First we have that the $|a_i\rangle = |\pm\rangle$ and the $|b_i\rangle = |S_x \pm\rangle = \frac{1}{\sqrt{2}}(|+\rangle \pm |-\rangle)$

$$\hat{U}=\begin{pmatrix} \langle a_1 |b_1\rangle & \langle a_1 |b_2\rangle \\ \langle a_2 |b_1\rangle & \langle a_2 |b_2\rangle \end{pmatrix}=\begin{pmatrix} \langle + |S_x; +\rangle & \langle + |S_x; -\rangle \\ \langle - |S_x; +\rangle & \langle - \mid S_x; -\rangle \end{pmatrix}=\frac{1}{\sqrt{2}}\begin{pmatrix} +1 & +1 \\ +1 & -1 \end{pmatrix} \quad \text{and} \quad \hat{U}^\dagger=\frac{1}{\sqrt{2}}\begin{pmatrix} +1 & +1 \\ +1 & -1 \end{pmatrix}$$

check unitarity

$$\hat{U}^\dagger\hat{U}=\frac{1}{\sqrt{2}}\begin{pmatrix} +1 & +1 \\ +1 & -1 \end{pmatrix} \frac{1}{\sqrt{2}}\begin{pmatrix} +1 & +1 \\ +1 & -1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} +2 & 0 \\ 0 & +2 \end{pmatrix}= \hat{1} \quad \text{it is}$$

check that

$$|b_j\rangle = \hat{U}\,|a_i\rangle \qquad \frac{1}{\sqrt{2}}\begin{pmatrix} +1 & +1 \\ +1 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix}= \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}\doteq|S_x; +\rangle \quad \text{and} \quad \frac{1}{\sqrt{2}}\begin{pmatrix} +1 & +1 \\ +1 & -1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix}= \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}\doteq|S_x; -\rangle \quad \text{good}$$

$\frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. That is we expect that the $|b_j\rangle$ are eigenkets of $\hat{U}^\dagger\hat{S}_x\hat{U}$ with the same eigenvalues as the $\hat{S}_x$ eigenvalues.

$$\hat{S}_x'=\hat{U}^\dagger\hat{S}_x\hat{U}=\frac{1}{\sqrt{2}}\begin{pmatrix} +1 & +1 \\ +1 & -1 \end{pmatrix}\frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} +1 & +1 \\ +1 & -1 \end{pmatrix}=\frac{1}{2}\frac{\hbar}{2}\begin{pmatrix} +1 & +1 \\ +1 & -1 \end{pmatrix}\begin{pmatrix} +1 & -1 \\ +1 & +1 \end{pmatrix}=\frac{1}{2}\frac{\hbar}{2}\begin{pmatrix} 2 & 0 \\ 0 & -2 \end{pmatrix}=\frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \text{so it}$$

works!

We should check $\text{Tr}(\hat{S}_x')=\text{Tr}(\hat{S}_x')$ or $\text{Tr}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}=\text{Tr}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}=0$ so it works

Example:

Diagonalize $\hat{X} = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$ So we need to find the eigenvalues and eigenkets of this matrix. The eigenkets will serve as the "new". The old basis is just $|\pm\rangle$

$$\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix}=\text{b}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} \quad \Longrightarrow \quad \begin{pmatrix} 1-b & -1 \\ -1 & 1-b \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix}=0 \quad \Longrightarrow \quad \det\begin{pmatrix} 1-b & -1 \\ -1 & 1-b \end{pmatrix}=0$$

$(1-b)^2\text{-}1=0$ b=0 or 2 are the eigenvalues for b=0 α-β=0 α=-β and using $\alpha^2+\beta^2=2$ we get that the eigenket is $\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$

for b=2 -α-β=0 and α=-β and using $\alpha^2+\beta^2=2$ we get that the eigenket is $\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$

So old basis is $|\pm\rangle$ the new basis is $\frac{1}{\sqrt{2}}$ ($|+\rangle+|-\rangle$) and $\frac{1}{\sqrt{2}}$ ($|+\rangle-|-\rangle$)

$\hat{U}=\frac{1}{\sqrt{2}}\begin{pmatrix}1&1\\1&-1\end{pmatrix}$ and $\hat{U}^\dagger=\frac{1}{\sqrt{2}}\begin{pmatrix}1&1\\1&-1\end{pmatrix}$

$\hat{U}^\dagger\,\hat{X}\,\hat{U}=\frac{1}{2}\begin{pmatrix}1&1\\1&-1\end{pmatrix}\begin{pmatrix}1&-1\\-1&1\end{pmatrix}\begin{pmatrix}1&1\\1&-1\end{pmatrix}=\frac{1}{2}\begin{pmatrix}1&1\\1&-1\end{pmatrix}\begin{pmatrix}0&2\\0&-2\end{pmatrix}=\frac{1}{2}\begin{pmatrix}0&0\\0&4\end{pmatrix}=\begin{pmatrix}0&0\\0&2\end{pmatrix}$

Note that the trace is 2 for the old and new basis and that for the new basis, the eigenvalues are down the diagonal.

Unitary Equivalent Observables

Theorem : If we have two basis sets connect by an operator $\hat{U}$ as $|b_i\rangle=\hat{U}\,|a_i\rangle$ then we may construct *a* unitary transform of A as $\hat{U}\,\hat{A}\,\hat{U}^{-1}$. $\hat{A}$ and $\hat{U}\,\hat{A}\,\hat{U}^{-1}$ are said to be unitary equivalent observables meaning that they have the *same sets of eigenvalues*.

Note first that the definition of $\hat{U}^{-1}$ is the inverse of $\hat{U}$ so that $\hat{U}^{-1}\hat{U}$=1

Proof of theorem: $\hat{A}\,|a_l\rangle=a_l|a_l\rangle \Longrightarrow \hat{A}\,\hat{U}^{-1}\,\hat{U}\,|a_l\rangle=a_l|\,a_l\rangle \Longrightarrow \hat{U}\,\hat{A}\,\hat{U}^{-1}\,\hat{U}\,|a_l\rangle=a_l\,\hat{U}\,|\,a_l\rangle \Longrightarrow \hat{U}\,\hat{A}\,\hat{U}^{-1}\,|b_l\rangle=a_l\,|\,b_l\rangle$

We can by definition write $\hat{B}\,|b_l\rangle=b_l\,|\,b_l\rangle$ and comparing this with $\hat{U}\,\hat{A}\,\hat{U}^{-1}\,|b_l\rangle=\hat{B}\,|b_l\rangle=a_l\,|\,b_l\rangle$ we recognize

that $\hat{B}$ and $\hat{U}\,\hat{A}\,\hat{U}^{-1}$ are simultaneously diagonalizable with the same eigenvalues. Often in the cases of physical interest, they are the same operator.

In our example $|b_i\rangle=|S_x\,\pm\rangle$ $\hat{B}=\hat{S}_x$ $|a_i\rangle=|\pm\rangle$ $\hat{A}=\hat{S}_z$ and $\hat{U}=\frac{1}{\sqrt{2}}\begin{pmatrix}+1&+1\\+1&-1\end{pmatrix}$ $\hat{U}^{-1}=\hat{U}^\dagger=\frac{1}{\sqrt{2}}\begin{pmatrix}+1&+1\\+1&-1\end{pmatrix}$

$\hat{U}\,\hat{S}_z\,\hat{U}^{-1}=\frac{1}{\sqrt{2}}\begin{pmatrix}+1&+1\\+1&-1\end{pmatrix}\frac{\hbar}{2}\begin{pmatrix}1&0\\0&-1\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}+1&+1\\+1&-1\end{pmatrix}=\frac{1}{2}\,\frac{\hbar}{2}\begin{pmatrix}+1&+1\\+1&-1\end{pmatrix}\begin{pmatrix}+1&+1\\-1&+1\end{pmatrix}=\frac{1}{2}\,\frac{\hbar}{2}\begin{pmatrix}0&2\\2&0\end{pmatrix}=\frac{\hbar}{2}\begin{pmatrix}0&1\\1&0\end{pmatrix}$

Now $\hat{B}=\hat{S}_x\doteq\begin{pmatrix}0&+1\\+1&0\end{pmatrix}$ and has eigenvalues $\pm\frac{\hbar}{2}$ with eigenvectors $\begin{pmatrix}1\\1\end{pmatrix}$ and $\begin{pmatrix}1\\-1\end{pmatrix}$ Lets check and see if these are eigenvectors of $\hat{U}\,\hat{S}_z\,\hat{U}^{-1}=\frac{\hbar}{2}\begin{pmatrix}0&1\\1&0\end{pmatrix}$ This is just $\hat{S}_x$ again, so its obvious that they are. As stated, the two operators $\hat{B}$ and $\hat{U}\,\hat{A}\,\hat{U}^{-1}$ are often the same operator in cases of interest.

So what this says in this case is that $\hat{S}_z$ and $\hat{S}_x=\hat{U}\,\hat{S}_z\,\hat{U}^{-1}$ are related by a unitary transformation $\hat{U}=\frac{1}{\sqrt{2}}\begin{pmatrix}+1&+1\\+1&-1\end{pmatrix}$ and have the same eigenvalues $\frac{\pm\hbar}{2}$. Now what is interesting is that we know what sort of transformation changes $\hat{S}_z$ to $\hat{S}_x$ - its a rotation. But is $\hat{U}$ really a rotation? Yes it is. It tells us how the 2 dimensional space of spin transforms under rotation in 3-space.

Note of interest:

The transformation that changes $\hat{S}_z$ to $\hat{S}_x$ is

$\hat{S}_i\to\hat{U}\,\hat{S}_i\,\hat{U}^{-1}$ is the same as $R_{ij}\hat{S}_j$ where R_{ij} is just a rotation. This can be done because the U's are just 2x2 matrices. But actually there are 2 U's that will do it. U, and -U this is just the double covering aspect of SU(2) to SO(3) which then means that fermions have a funny thing that a rotation in 2π does not bring you back to the same thing but you have to go through 4π.

