Notes for Quantum Mechanics

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Lecture 7- Matrix Representations

There an easy way to work with operators and bras and kets which we will utilize especially for spin 1/2 systems. It becomes a bit cumbersome for other systems, but it is useful for any discreet set of eigenfunctions. This is the matrix representation of an operator.

A first critical thing to remember is that you must pick a basis in order to have a matrix representation.

Lets first find the matrix representation of an operator $\hat{X}$ where we have picked a basis set of eigenkets we will denote as $|a\rangle$

Now ley me clarify some notation I will use. $|a\rangle$ will denote eigenkents of the operator $\hat{A}$.

First I will multiply $\hat{X}$ by $\hat{1}$ a couple times where I recall that $\hat{1} = \sum_i |a_i\rangle \langle a_i|$ note that I am very careful with the indices

$\hat{X} = \hat{1}\,\hat{X}\,\hat{1} = \sum_i |a_i\rangle \langle a_i|\,\hat{X}\,\sum_j |a_j\rangle \langle a_j| = \sum_{i,j} |a_i\rangle \langle a_i|\,\hat{X}\,|a_j\rangle \langle a_j|$ - now lets look at the term in the middle of this expression $\langle a_i|\,\hat{X}\,|a_j\rangle$

Now lets make a matrix out of this so we write out all the possible terms. We will let the i index denote the rows and the j index denote the columns. The funny equal sign $\doteq$ will mean a matrix representation which also means that we have picked a basis Lets pretend that the indices run from 1 to3, that is that there are three basis vectors. Then we can write

$$\hat{X} \doteq \begin{pmatrix} \langle a_1|\,\hat{X}\,|a_1\rangle & \langle a_1|\,\hat{X}\,|a_2\rangle & \langle a_1|\,\hat{X}\,|a_3\rangle \\ \langle a_2|\,\hat{X}\,|a_1\rangle & \langle a_2|\,\hat{X}\,|a_2\rangle & \langle a_2|\,\hat{X}\,|a_3\rangle \\ \langle a_3|\,\hat{X}\,|a_1\rangle & \langle a_3|\,\hat{X}\,|a_2\rangle & \langle a_3|\,\hat{X}\,|a_3\rangle \end{pmatrix} \tag{1}$$

Now lets recall a couple of relationships from before.

$\langle a_i \mid \hat{X} \mid a_j\rangle = \langle a_j \mid \hat{X}^\dagger \mid a_i\rangle^*$ (lecture 6 eqn 32)

so if $\hat{X}$ was Hermitian, i.e. $\hat{X} = \hat{X}^\dagger$ then $\langle a_i \mid \hat{X} \mid a_j\rangle = \langle a_j \mid \hat{X} \mid a_i\rangle^*$ (2)

Now let think of what this means for the matrix representation of $\hat{X}$
It means if $\hat{X}$ is hermitian, then the matrix is equal to its complex conjugate transposed. This is the definition of Hermitian for a matrix (3)
Does this sound familiar to those who have taken linear algebra?

Now lets see if we can also find a representation of the bra's and kets which can work with this matrix representation of the operator.

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$|\gamma\rangle = \hat{X}\,|\alpha\rangle$ then

$\langle a_j|\gamma\rangle = \langle a_j \mid \hat{X} \mid \alpha\rangle = \langle a_j \mid \hat{X}\,\hat{1} \mid \alpha\rangle = \langle a_j \mid \hat{X} \sum_i |a_i\rangle\langle a_i \mid \alpha\rangle = \sum_i \langle a_j \mid \hat{X}\,|a_i\rangle\langle a_i \mid \alpha\rangle$

We see here the matrix representation of $\hat{X}$ in the first term and we take the second term to be the representation of the ket

Its a column of numbers where the i represents the row number $|\alpha\rangle \doteq \begin{pmatrix} \langle a_1 \mid \alpha\rangle \\ \langle a_2 \mid \alpha\rangle \\ \langle a_3 \mid \alpha\rangle \end{pmatrix}$ (4)

For a bra $\langle\alpha| \doteq (\langle\alpha \mid a_1\rangle \;\; \langle\alpha \mid a_2\rangle \;\; \langle\alpha \mid a_3\rangle)$ (5)

Now for those who know some linear algebra, you see that the rules of matrix multiplication (I will go over these) etc hold. Remember though, its really a shortcut for writing out the sums. If you get confused, write out the sums.

Lets represent $\hat{A}$ (remember $\langle a_i|$ are the eigenvalues of $\hat{A}$)

$\hat{A} = \hat{1}\hat{A}\hat{1} = \sum_i |a_i\rangle\langle a_i|\,\hat{A} \sum_j |a_j\rangle\langle a_j| = \sum_{i,j} |a_i\rangle\langle a_i|\,\hat{A}|a_j\rangle\langle a_j| = \sum_{i,j} |a_i\rangle\, a_j\, \langle a_i|a_j\rangle\langle a_j|$
$= \sum_{i,j} |a_i\rangle\, a_j\, \delta_{ij}\, \langle a_j| = \sum_i a_i\, |a_i\rangle\langle a_i| = \sum_i a_i \hat{\Lambda}_i$

where we remember the projection operator $\hat{\Lambda} = |a_i\rangle\langle a_i|$

Let me give a number to this
$\hat{A} = \sum_i a_i\, |a_i\rangle\langle a_i| = \sum_i a_i \hat{\Lambda}_i$ (6)

We can see that the matrix for $\hat{A}$ IN THIS REPRESENTATION (where we use the eigenkets of $\hat{A}$ as a basis) is diagonal

$\hat{A} \doteq \begin{pmatrix} a_1 & 0 & 0 \\ 0 & a_2 & 0 \\ 0 & 0 & a_3 \end{pmatrix}$ (7)

A point: one has to pick an order for the basis vectors in the matrix representation. [e.g. in cartesian coordinates, we always go in the order x, y, z.

Some brief notes about matrices

See a good tutorial here http://people.hofstra.edu/faculty/Stefan_Waner/RealWorld/tutorialsf1/frames3_2.html - do this tutorial if you are rusty. You will be glad you did.

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