Quantum Mechanics

Introduction

WP Status

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This document contains record of my understanding of Chapter 1 Fundamental Concepts, from J.J. Sakurai.

Areas marked with a **Doubt** or **Find out** are ones I am not absolutely clear about. Perhaps reiterating later would help.

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1 Introduction

1.1 Stern Gerlach

Silver atom has 47 electrons, of which 46 are paired. The 47^{th} has a spin, but no orbital-angular momentum (because it's an s electron). **Doubt** In accordance with the book, and I quote 'The 47 electrons are attached to the nucleus, which is 2×10^5 times heavier than the electron; as a result, the heavy atom as a whole possesses a magnetic moment equal to the spin magnetic moment of the 47^{th} electron'. Does that mean that if the electrons were comparable in mass with the nucleus, we would couldn't have claimed that the magnetic moment of the atom is same as that of the electron? I can not see the co-relation between spin angular moment and mass. Also, why is the nuclear spin ignored and how is it justified?

Force on a magnetic dipole is given by $\boldsymbol{F} = \nabla(\boldsymbol{\mu}.\boldsymbol{B})$. For a Magnetic field varying along z only, we therefore have

$$F_z = \mu_z \frac{\partial B_z}{\partial z} \tag{1}$$

So we would expect the Stern Gerlach experiment to split the two beams into two, along the z axis. And this is what was observed. However things get interesting when we cascade these experiments. The beam from the $\hat{\boldsymbol{z}}+$ from the SG $\hat{\boldsymbol{z}}$ apparatus is allowed to go through the SG $\hat{\boldsymbol{z}}$ again, and we observe only the S $\hat{\boldsymbol{z}}+$ component. Which is again as expected. However, if the $\hat{\boldsymbol{z}}+$ beam is passed through an SG $\hat{\boldsymbol{x}}$ apparatus, we get both $\hat{\boldsymbol{x}}+$ and $\hat{\boldsymbol{x}}-$ beams. Now also, one may be able to rationalize the result by saying the incident beam had both $\hat{\boldsymbol{z}}\pm$ and $\hat{\boldsymbol{x}}\pm$ and after blocking $\hat{\boldsymbol{z}}-$, we had $\hat{\boldsymbol{z}}+$ and $\hat{\boldsymbol{x}}\pm$. Then on splitting by SG $\hat{\boldsymbol{x}}$, we got $\hat{\boldsymbol{x}}\pm$. However, this gets into trouble with the final blow. Here's the setup. SG $\hat{\boldsymbol{z}}$, blocked $\hat{\boldsymbol{z}}-$, SG $\hat{\boldsymbol{x}}$, blocked $\hat{\boldsymbol{x}}-$, SG $\hat{\boldsymbol{z}}$, and we get $\hat{\boldsymbol{x}}\pm$!

The book at this stage, points out the following

- Spin components along $\hat{\boldsymbol{z}}$ and $\hat{\boldsymbol{y}}$ can't be measured simultaneously
- This more *precisely* means that selection of the $\hat{\boldsymbol{x}}$ component by the SG $\hat{\boldsymbol{x}}$ apparatus, removes any information about the $\hat{\boldsymbol{z}}$ component.

The book then gives an analogy with the book, which by itself is substantially clear, though long and has been omitted from the discussion.

1.2 Kets Bras and Operators

1.2.1 Ket Space

State of a system is represented by a *state vector*, which is known as *ket*, and is denoted by $|\alpha>$. The state vector is postulated to contains all information retrievable about the system. Following are properties of kets, arbitrarily defined to be true at this stage

1. $|\alpha> + |\beta> = |\gamma>$
2. $c|\alpha> = |\alpha> c$, where c is complex and if $c = 0$, the resultant is a *null ket*.
3. *Observables* are represented by *operators* which act on kets as $A.(|\alpha>) = A|\alpha>$
   (a) in general, $A|\alpha>$ is not of the type $c|\alpha>$ (where c is complex)
   (b) for *eigenkets* of A, the operation is always a scalar multiple of the eigenket and the scalar is called the *eigenvalue*
   (c) nomenclature: it is typical to represent eigenkets with eigenvalues $a', a'', a''', ...$ by $|a'>, |a''>, |a'''>, ...$ respectively.
   (d) familiar rules related to vector spaces: An N-dimensional vector space is spanned by the N eigenkets of the observable A.

1.2.2 Bra Space and Inner Products

Bra space is 'dual to' the ket space. Why this must be introduced is a mystery as of now, but it should become clear soon enough.

1. Postulate: For every ket, $|\alpha>$ in the ket space, $\exists$ a bra $<\alpha|$ in the bra space.
   (a) $|\alpha> \underset{\text{DC}}{\longleftrightarrow} <\alpha|$
   (b) $|\alpha> + |\beta> \underset{\text{DC}}{\longleftrightarrow} <\alpha| + <\beta|$
   (c) $c_\alpha|\alpha> + c_\beta|\beta> \underset{\text{DC}}{\longleftrightarrow} c_\alpha^* <\alpha| + c_\beta^* <\beta|$
2. The bra space is spanned by *eigenbras*, the bras dual to the eigenkets
3. *Inner product* is defined as $\langle\beta|\alpha\rangle = (\langle\beta|)(|\alpha\rangle)$, bra(c)ket! The answer is a complex number.
   (a) Postulate: $\langle\beta|\alpha\rangle = \langle\alpha|\beta\rangle^*$
   Easy deduction: $\Rightarrow \langle\alpha|\alpha\rangle$ is a real number.
   (b) Postulate of *Positive Definite Metric*: $\langle\alpha|\alpha\rangle \geq 0$, where equality holds iff $|\alpha\rangle$ is a null ket.
4. Iff $\langle\alpha|\beta\rangle = 0$, then $|\alpha\rangle$ and $|\beta\rangle$ are *orthogonal*.
5. *Norm* of a ket $|\alpha\rangle$ is given by $\sqrt{\langle\alpha|\alpha\rangle}$
6. A *Normalized ket* is given by
$$|\tilde{\alpha}\rangle = \frac{1}{\sqrt{\langle\alpha|\alpha\rangle}}|\alpha\rangle$$
   so that for a normalized ket, we get $\langle\tilde{\alpha}|\tilde{\alpha}\rangle = 1$

1.2.3 Operators

1. An operator (represented by X, Y etc.) act on kets from the left to result in another ket. They act on bras from the right.
   (a) Two operators X and Y are equal iff $\forall\ |\alpha\rangle$, we have $X|\alpha\rangle = Y|\alpha\rangle$
   (b) X is a *null operator* iff $X|\alpha\rangle = 0 \ \forall\ |\alpha\rangle$
2. Addition of Operators
   (a) For operators, addition operations are commutative and associative
   (b) Operators are also linear, viz. $X(c_\alpha|\alpha\rangle + c_\beta|\beta\rangle) = c_\alpha X|\alpha\rangle + c_\beta X|\beta\rangle$, except for an exception of the time-reversal operator
3. Relations between Operation on Bras and Kets
   (a) $X|\alpha\rangle \underset{\text{DC}}{\not\longleftrightarrow} \langle\alpha|X$ in general
   (b) The *Hermitian adjoint*, $X^\dagger$ is defined as $X|\alpha\rangle \underset{\text{DC}}{\longleftrightarrow} \langle\alpha|X^\dagger$
   (c) An operator is *Hermitian* iff $X = X^\dagger$
4. Multiplication of Operators
   (a) Multiplication of operators is not commutative, but it is associative
   Associativity holds good for all legal multiplications, viz. the ones defined here
   (b) $X(Y|\alpha\rangle) = (XY)|\alpha\rangle = XY|\alpha\rangle$ and similarly $(\langle\beta|X)Y = \langle\beta|(XY) = \langle\beta|XY$
   (c) $(XY)^\dagger = Y^\dagger X^\dagger$

   Proof.

   We know $(XY)|\alpha\rangle \underset{\text{DC}}{\longleftrightarrow} \langle\alpha|(XY)^\dagger$
   We also know $(Y|\alpha\rangle) \underset{\text{DC}}{\longleftrightarrow} (\langle\alpha|Y^\dagger)$
   Let $Y|\alpha\rangle = |\beta\rangle$
   $\Rightarrow Y|\alpha\rangle = |\beta\rangle \underset{\text{DC}}{\longleftrightarrow} \langle\beta| = \langle\alpha|Y^\dagger$
   Then $X|\beta\rangle \underset{\text{DC}}{\longleftrightarrow} \langle\beta|X^\dagger$
   $\Rightarrow XY|\alpha\rangle \underset{\text{DC}}{\longleftrightarrow} \langle\alpha|Y^\dagger X^\dagger$

   □

5. *Outer Product* is defined as $(|\beta\rangle)(\langle\alpha|) = |\beta\rangle\langle\alpha|$.
   (a) This is not a number, it's an operator.

   Proof. Consider $(|\beta\rangle\langle\alpha|)|\gamma\rangle$ which by associativity, we can write as $|\beta\rangle(\langle\alpha||\gamma\rangle) = |\beta\rangle(\langle\alpha|\gamma\rangle)$ □

   (b) If $X = |\beta\rangle\langle\alpha|$, then $X^\dagger = |\alpha\rangle\langle\beta|$

Proof. $X = |\beta\rangle\langle\alpha|$, so
$X|\gamma\rangle = (|\beta\rangle\langle\alpha|).|\gamma\rangle = |\beta\rangle(\langle\alpha|\gamma\rangle) \underset{\text{DC}}{\longleftrightarrow} \langle\beta|(\langle\alpha|\gamma\rangle)^* = (\langle\gamma|\alpha\rangle)\langle\beta| = \langle\gamma|(|\alpha\rangle\langle\beta|) = \langle\gamma|X^\dagger$ □

6. Since $(\langle\beta|)(X|\alpha\rangle) = (\langle\beta|X)(|\alpha\rangle)$, we denote it by a simpler notation $\langle\beta|X|\alpha\rangle$.
Now we claim

$$\langle\beta|X|\alpha\rangle = \langle\alpha|X^\dagger|\beta\rangle^* \tag{2}$$

Proof. We know that $\langle a|b\rangle \underset{\text{DC}}{\longleftrightarrow} \langle b|a\rangle$ and that $X|\alpha\rangle \underset{\text{DC}}{\longleftrightarrow} \langle\alpha|X^\dagger$. Let $X|\alpha\rangle = |\gamma\rangle$ thus

$$\begin{aligned}\langle\beta|X|\alpha\rangle &= (\langle\beta|)(|\gamma\rangle)\\ &= \langle\beta|\gamma\rangle\\ &= \langle\gamma|\beta\rangle^*\\ &= ((\langle\alpha|X^\dagger)(|\beta\rangle))^*\\ &= \langle\alpha|X^\dagger|\beta\rangle^*\end{aligned}$$

□

And when X is hermitian, viz. $X = X^\dagger$, we have $\langle\beta|X|\alpha\rangle = \langle\alpha|X|\beta\rangle^*$

1.3 Base Kets and Matrix Representations

1.3.1 Eigenkets of an Observable

Let us first talk about Hermitian Operators and we will then justify the use of the word observable.

Theorem. *The eigenvalues of a Hermitian operator A are real*

Proof. Consider a Hermitian operator A. We have, following from the previous sections,

$$A|a'\rangle = a'|a'\rangle \tag{3}$$

where $a', a'', a''', ...$ are eigenvalues for A, and $|a'\rangle, |a''\rangle, |a'''\rangle, ...$ are the corresponding eigenkets.
Now since A is hermitian, we know

$$\begin{aligned}A|a'\rangle &\underset{\text{DC}}{\longleftrightarrow} \langle a'|A\\ \Rightarrow a'|a'\rangle &\underset{\text{DC}}{\longleftrightarrow} a'^*\langle a'| = \langle a'|A\end{aligned}$$

So in general, we also have

$$\langle a''|A = a''^*\langle a''| \tag{4}$$

Now we simply multiply the first relation with $|a''\rangle$ from the left and the other with $|a'\rangle$ from the right to obtain

$$\langle a''|A|a'\rangle = a'\langle a''|a'\rangle \tag{5}$$
$$\langle a''|A|a'\rangle = a''^*\langle a''|a'\rangle \tag{6}$$

On subtraction we get

$$(a' - a''^*)\langle a''|a'\rangle = 0 \tag{7}$$

We are almost there. Now consider the case when $a' \neq a''$, so that $a' - a''^* \neq 0$ in general. Then for the LHS to be zero, we must have $\langle a''|a'\rangle = 0$. So this proves that all eigenkets of A are mutually orthogonal. Next, if $a' = a''$, then since $\langle a'|a'\rangle \geq 0$, and the equality holds only if $|a'\rangle$ is a null ket, which it is not, therefore we must have $a' - a'^* = 0 \Rightarrow a'$ is real. □

It is conventional to normalize the eigenkets to make them into an *orthonormal* set as

$$\langle a''|a'\rangle = \delta_{a'',a'} \tag{8}$$

where $\delta_{a'',a'}$ represents the Kronecker Delta function.
Further, from our assumption, the eigenkets span the eigenspace for a given operator A.

1.3.2 Eigenkets as Base Kets

Since the entire ket space can be represented by the eigenkets of A, we thus have

$$|\alpha\rangle = \sum_{a'} c_{a'}|a'\rangle \tag{9}$$

To find the co-efficient $c_{a''}$, we just left multiply, both sides of the equation with $\langle a''|$ to get

$$\langle a''|\alpha\rangle = c_{a''} \tag{10}$$

(we've used the orthonormality of the eigenkets here)
We thus also have

$$\begin{aligned}
|\alpha\rangle &= \sum_{a'} |a'\rangle\langle a'|\alpha\rangle && (11)\\
&= \sum_{a'} (|a'\rangle\langle a'|)|\alpha\rangle && (12)\\
\Rightarrow \sum_{a'} |a'\rangle\langle a'| = 1 & && \text{(as } |\alpha\rangle \text{ is arbitrary)} \quad (13)
\end{aligned}$$

Equation 13 is known as the *completeness relation* or *closure*.
Consider the following application of the completeness relation;

$$\begin{aligned}
\langle\alpha|\alpha\rangle &= |\alpha\rangle \left(\sum_{a'} \langle a'||a'\rangle\right) \langle\alpha| && (14)\\
&= \sum_{a'} (\langle a'|\alpha\rangle^2) = \sum_{a'} c_{a'}^2 && (15)\\
&= 1 && \text{(if } |\alpha\rangle \text{ is normalized)} \quad (16)
\end{aligned}$$

Which easily proves a remarkable relation, with a smell of similarity with probabilities.
We now declare the outer product $|a'\rangle\langle a'|$ as the *projection operator* along the ket $|a'\rangle$ and denote it by $\Lambda_{a'}$. Equation 13 can now be expressed as

$$\sum_{a'} \Lambda_{a'} = 1 \tag{17}$$

We now justify the word 'projection';

$$\Lambda_{a'}|\alpha\rangle = |a'\rangle\langle a'|\alpha\rangle = c_{a'}|a'\rangle \tag{18}$$

1.3.3 Matrix Representations

We can write the operator X as

$$X = \sum_{a''}\sum_{a'} |a''\rangle\langle a''|X|a'\rangle\langle a'| \tag{19}$$

by invoking the closure property as described earlier.

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If there're N eigenkets for the ketspace of X, thus there would be N^2 $\langle a''|X|a'\rangle$ elements. These terms can be written explicitly in an $N \times N$ matrix, which *represents* the operator.

$$X \doteq \begin{pmatrix} \langle a^{(1)}|X|a^{(1)}\rangle & \langle a^{(1)}|X|a^{(2)}\rangle & \langle a^{(1)}|X|a^{(3)}\rangle & .. & .. \\ \langle a^{(2)}|X|a^{(1)}\rangle & \langle a^{(2)}|X|a^{(2)}\rangle & \langle a^{(2)}|X|a^{(3)}\rangle & .. & .. \\ \langle a^{(3)}|X|a^{(1)}\rangle & \langle a^{(3)}|X|a^{(2)}\rangle & \langle a^{(3)}|X|a^{(3)}\rangle & .. & .. \\ .. & .. & .. & . & \\ .. & .. & .. & & . \end{pmatrix} \tag{20}$$

We already know from Equation 2 then, that

$$\langle a''|X|a'\rangle = \langle a'|X^\dagger|a''\rangle^* \tag{21}$$

Uncertain (not the uncertainty principle) [Given the matrix form of an operator, we can write the matrix for it's Hermitian adjoint by taking the complex conjugated transpose of the given matrix, with $X^\dagger$ instead of X, as described by the equation.]
Interestingly enough, the definition conforms with the laws of matrix multiplication to yield the corresponding operator multiplication. Take for instance

$$Z = XY \tag{22}$$

Each element in the matrix representation of Z can then be written as

$$\langle a^{\text{row}}|XY|a^{\text{column}}\rangle \tag{23}$$

We can introduce using closure the following without affecting equality

$$= \sum_{a'} \langle a^{\text{row}}|X|a'\rangle\langle a'|Y|a^{\text{column}}\rangle \tag{24}$$

Which is precisely the matrix multiplication operation.

Let us now talk about the matrix represenation of a ket $|\alpha\rangle$, begin acted upon by an operator like so

$$|\gamma\rangle = X|\alpha\rangle \tag{25}$$

Now to find the co-efficients of $|\gamma\rangle$ with respect to the eigenkets, we simply need to multiply the equation on the left by $\langle a'|$ to obtain

$$\langle a'|\gamma\rangle = \langle a'|X|\alpha\rangle \tag{26}$$

We again use the same trick of closure, and rewrite the equation as

$$\langle a'|\gamma\rangle = \sum_{a'} \langle a'|A|a''\rangle\langle a''||\alpha\rangle \tag{27}$$

A closer look confirms the hunch that this is a square matrix multiplied by a row matrix. If we define the following representations

$$|\gamma\rangle \doteq \begin{pmatrix} \langle a^{(1)}|\gamma\rangle \\ \langle a^{(2)}|\gamma\rangle \\ \langle a^{(3)}|\gamma\rangle \\ .. \end{pmatrix} \tag{28}$$

$$|\alpha\rangle \doteq \begin{pmatrix} \langle a^{(1)}|\alpha\rangle \\ \langle a^{(2)}|\alpha\rangle \\ \langle a^{(3)}|\alpha\rangle \\ .. \end{pmatrix} \tag{29}$$

then the operation of X on $|\alpha\rangle$ is simply a matrix multiplication;

$$|\gamma\rangle = X|\alpha\rangle \tag{30}$$

Similarly, we have for a bra, given

$$\langle\gamma| = \langle\alpha|X \tag{31}$$

the following

$$\langle\gamma|a'\rangle = \sum_{a''}\langle\alpha|a''\rangle\langle a''|X|a'\rangle \tag{32}$$

This looks like a row (not a column) multiplied by a square matrix, which similar to kets, inspires the following representation definitions, for it to indeed be the case

$$\langle\gamma| \doteq \left(\langle\gamma|a^{(1)}\rangle, \langle\gamma|a^{(2)}\rangle, \langle\gamma|a^{(3)}\rangle, ...\right) = \left(\langle a^{(1)}|\gamma\rangle^*, \langle a^{(2)}|\gamma\rangle^*, \langle a^{(3)}|\gamma\rangle^*, ...\right) \tag{33}$$

and similarly

$$\langle\alpha| \doteq \left(\langle a^{(1)}|\alpha\rangle^*, \langle a^{(2)}|\alpha\rangle^*, \langle a^{(3)}|\alpha\rangle^*, ...\right) \tag{34}$$

With that done, let's talk about the inner product $\langle\beta|\alpha\rangle$ and see if it is consistent with our representations of Bras and Kets as described here. We have

$$\langle\beta|\alpha\rangle = \langle\beta||\alpha\rangle \tag{35}$$

$$= \sum_{a'}\langle\beta||a'\rangle\langle a'||\alpha\rangle \tag{36}$$

which is precisely, the row representation of $\langle\beta|$ times the column representation of $|\alpha\rangle$. Also observe if we multiply corresponding representation of $\langle\alpha|$ with that of $|\beta\rangle$, we obtain the complex conjugate of $\langle\beta|\alpha\rangle$ as represented above; consistent with the fundamental property of the inner product.

The last representation of the section, will be that of the outer product (an operator), which is given by an $N \times N$ matrix, as we now multiply a column matrix $N \times 1$ with a row matrix $1 \times N$. We thus, quite simply have

$$|\beta\rangle\langle\alpha| \doteq \begin{pmatrix} \langle a^{(1)}|\beta\rangle^*\langle a^{(1)}|\alpha\rangle & \langle a^{(2)}|\beta\rangle^*\langle a^{(1)}|\alpha\rangle & \langle a^{(3)}|\beta\rangle^*\langle a^{(1)}|\alpha\rangle & .. \\ \langle a^{(1)}|\beta\rangle^*\langle a^{(2)}|\alpha\rangle & \langle a^{(2)}|\beta\rangle^*\langle a^{(2)}|\alpha\rangle & \langle a^{(3)}|\beta\rangle^*\langle a^{(2)}|\alpha\rangle & .. \\ .. & .. & .. & \end{pmatrix} \tag{37}$$

(Note: The star is for complex conjugation, not multiplication!)
If the operator is observable, say A, and we try to represent it using it's own eigenkets, then we get

$$A = \sum_{a'}\sum_{a''}|a''\rangle\langle a''|A|a'\rangle\langle a'| \tag{38}$$

In here, observe that $|a''\rangle$ can be thought of as representing a column matrix of $1 \times N$, and $\langle a'|$ as a row matrix of $N \times 1$, and therefore $\langle a''|A|a'\rangle$ should be represented by an $N \times N$ square matrix. Since $|a'\rangle$ and $|a''\rangle$ are eigenkets, thus we have

$$\begin{aligned}\langle a''|A|a'\rangle &= \langle a''|a'|a'\rangle && (39)\\ &= \langle a''||a'\rangle a' && (40)\\ &= \langle a'|a'\rangle a'\delta_{a',a''} && (41)\\ &= a'\delta_{a',a''} && (42)\end{aligned}$$

which basically shows the matrix is diagonal. Now going back, we have

$$\begin{aligned}A &= \sum_{a'}\sum_{a''}|a''\rangle a'\delta_{a',a''}\langle a'| = \sum_{a'}\sum_{a''}|a'\rangle a'\delta_{a',a''}\langle a'| && (43)\\ &= \sum_{a'}\sum_{a''}a'|a'\rangle\langle a'|\delta_{a',a''} = \sum_{a'}\sum_{a''}a'\Lambda_{a'}\delta_{a',a''} && (44)\\ &= \sum_{a'}a'\Lambda_{a'} && (45)\end{aligned}$$
