2.6 Representation Theory

2.6.1 Introductory Linear Algebra

1. Revise Sections II and IIIand do the following homework problems
   (a) **Write down all the dyadic products** $\vec{i}\vec{i}^\dagger$, $\vec{i}\vec{j}^\dagger$, $\vec{i}\vec{k}^\dagger$, $\vec{j}\vec{i}^\dagger$, $\vec{j}\vec{j}^\dagger$, $\vec{j}\vec{k}^\dagger$, $\vec{k}\vec{i}^\dagger$ $\vec{k}\vec{j}^\dagger$, $\vec{k}\vec{k}^\dagger$
   (b) **Homework: Show that:**

$$\vec{i}\vec{i}^\dagger + \vec{j}\vec{j}^\dagger + \vec{k}\vec{k}^\dagger = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{2.6.1}$$

   The matrix on the right hand side in this equation is called the identity or unit matrix. This relation is called the *resolution of the identity* and we will have a great deal of need for this expression.

2. The resolution of the identity is also known as the completeness relation.

3. Any vector can be written as a linear combination of an *ortho-normal* and *complete* set of vectors. As the set $\hat{i}$, $\hat{j}$ and $\hat{k}$ are *ortho-normal* and *complete* (as seen in point 1b) it comes as no surprise to us that any vector in three-dimension can be written as a linear combination of these vectors.

4. **Homework:** Show that the spin states SG_z^+ and SG_z^- (we learn a better way to represent these states soon) form a complete orthonormal set. (Use the analogy to the x- and y-filters.) Hint: This question is simpler than you might think!!

2.7 Dirac Notation

1. The discussion in the linear algebra handouts is heavily couched in the 3-dimensional space. However, you will note that there is no restriction as such, on the algebra. All of what we had learned (dot products, dyads, resolution of identity, etc.) could very well be true for vectors in say 4-dimensions (or (4 $\times$ 1) matrices and their (1 $\times$ 4) dual counterparts) and matrices in 4-dimensions (*i.e.* (4 $\times$ 4) matrices). It would be very difficult (!!!!) for me to draw something in 4-dimensions, but in this lecture we will see how we can think in 4 or more dimensions.

2. While constructing the *analogy of the Stern-Gerlach spin states to polarized light* we learned that the polarized light can be treated using vectors and the Stern-Gerlach states are analogous to these. In a quantum mechanical system there will in general be a large number of such states. There should be a way for us to generalize the theory of vectors to arbitrary dimensions. This is what we will look into next.

3. Why arbitrary dimensions? We already saw that *four real dimensions* or two complex dimension were required to represent the spin states. See the Stern Gerlach handout.

 ©2014, Srinivasan S. Iyengar (instructor)

4. To make it to n-dimensions, the first thing we will do is introduce a new set of notations. The notation in the previous subsection is very nice for 3-dimensional space but turns out to be highly cumbersome in n-dimensions. The notation we are about to introduce is that due to Dirac, and hence is called the Dirac notation.

    - A vector in n-dimensions will be represented by the object: $|i\rangle$, and we will call this a *ket*, or a *ket*-vector.
    - The dual space analog of the *ket*, $|i\rangle$, is called the *bra* and is represented by $\langle i|$. (**Note: The *ket*, $|i\rangle$, is a vector in n-dimensions. A corresponding vector in 3-dimensions we represented as $\vec{i}$, earlier. The *bra*, $\langle i|$, is the dual-space analogue of the *ket*. In 3-dimensions we represented the dual space analogue of $\vec{i}$ as $\vec{i}^\dagger$. It is useful to keep these straight in our mind, so we do not get lost while we walk up to n-dimensions.**)
    - The reason for these peculiar names (*bra* and *ket*) is, the "dot" product is now a product of the *bra* and the *ket* and hence is the *bra-ket* :-) $\langle i| \, |i\rangle$, analogous to $\vec{i}^\dagger\vec{i}$ in 3-dimensions, which is a number like $\langle i| \, |i\rangle$. (In practice we choose to be lazy and drop one of the vertical bars in the middle of the *bra-ket* and represent it as $\langle i| \, i\rangle$.)
    - The outer product or the dyadic product that we made so much fuss about in the previous subsection if a *ket* $\times$ a *bra*. **Why?** Because the dyadic product in 3-dimensions (see Eq. (III.0.1)) is a vector times its dual space analogue, *for example* $\vec{i}\vec{k}^\dagger$.
    - **And the vector in n-dimensions is a *ket*, and its dual space analogue is the *bra*.** So the dyadic product is $|i\rangle \langle i|$.

5. This notation is due to P. A. M. Dirac in the late 1920s and hence is called the Dirac notation.

6. The resolution of identity in Dirac's notation.

    - Do we recall what a complete set of vectors in 3-dimensions is? A set of vectors that are *ortho-normal* and a set of vectors that obey the resolution of identity, Eq. (2.6.1). So, as we saw in the previous section, $\hat{i}$, $\hat{j}$ and $\hat{k}$ form a complete set.
    - In more simple terms, what we mean by $\hat{i}$, $\hat{j}$ and $\hat{k}$ form a complete set in 3-dimensions is that any vector in three-dimensions can be written as a linear combination (as in Eq. (II.0.1)) of $\hat{i}$, $\hat{j}$ and $\hat{k}$. (**Homework: By extension, could you comment on why Eqs. 2.4.13, 2.4.14 2.4.17, and (2.4.18), might actually make sense based on what we have noted here? Utilize your result from the homework problem on page 32.**)
    - Here we want to see what the corresponding set of rules would be for n-dimensions. And as we will see below these set of rules are very similar to what we have in 3-dimensions.
    - But, first, what does the number n in $\{|n\rangle\}$ mean? It could, for example, be a number-

 ©2014, Srinivasan S. Iyengar (instructor)

ing scheme:

$$|m\rangle \equiv \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix} \tag{2.7.2}$$

where the 1 is on the m-th position. n columns in all. So $|m\rangle$ in the equation above is a ($n\times$ 1) matrix that has all zeroes except at the m-th position.

- **Note: Eq. (2.7.2) is just an example of what $|m\rangle$ can be. More generally, it is just some vector in n-dimensions.**
- Now we are in a position to generalize the resolution of identity or completeness relation that we derived earlier for the 3-dimensional case. The corresponding relation for n-dimensions is:

$$\sum_{i=1}^{n} |i\rangle \langle i| = I \tag{2.7.3}$$

where the right hand side is the identity matrix. You can see that for n=3, the left hand side in Eq. (2.7.3) has three terms just like in Eq. (2.6.1). *In fact Eq. (2.7.3) is identical to Eq. (2.6.1) in three-dimensions* !!! In higher dimensions Eq. (2.7.3) provides us an additional tool.

- **Homework:**
  (a) Can you show that $|SG_z^+\rangle$ and $|SG_z^-\rangle$ (notice the new *ket* notation being used here to describe these states) form a complete set? How about $|SG_x^+\rangle$ and $|SG_x^-\rangle$? How about $\left|SG_y^+\right\rangle$ and $\left|SG_y^-\right\rangle$? Show your results.

7. The n-dimensional space that we just spoke about, is also called the **Hilbert space** in quantum mechanics. (After D. Hilbert a famous mathematician in the 20 century.)

8. Why do we care about all this?

9. These are the necessary mathematical tools we need to develop quantum mechanics.

10. Consider the Stern-Gerlach experiments we studied earlier. We may now choose to the denote the SG_z^+ state by the *ket* $|SG_z^+\rangle$. Why is this interesting? Because now we see that a state in quantum mechanics such as $|SG_z^+\rangle$ is essentially a vector in some n-dimensional space (the Hilbert space).

11. And since $|SG_z^+\rangle$ is a *ket*, it can be written as a linear combination of some complete set of *kets* like in Eq. (2.7.2). That is,

$$\left|SG_z^+\right\rangle \equiv \left\{\sum_{i=1}^{n} |i\rangle \langle i|\right\} \left|SG_z^+\right\rangle = \sum_{i=1}^{n} |i\rangle \langle i| \; SG_z^+\right\rangle = \sum_{i=1}^{n} c_i \, |i\rangle \tag{2.7.4}$$

 ©2014, Srinivasan S. Iyengar (instructor)

where $c_i = \langle i| SG_z^+\rangle$ are just numbers (*but they could be complex* !!). Note, we have introduced "1", *i.e.* the resolution of the identity of Eq. (2.7.3) in the second part of Eq. (2.7.4). Physically c_i are the "dot" product or inner product or *bra-ket* of $\langle i|$ with $|SG_z^+\rangle$. The c_i are just numbers and note the similarity between the above equation and the first equation in the linear algebra handout Eq. (II.0.1). x, y and z are also just numbers in Eq. (II.0.1).)

12. In addition, Eq. (2.7.4) tells us how to "change basis" from $|SG_z^+\rangle$ to $\{|i\rangle\}$. Can we visualize change of basis in three-dimensions?

2.8 So what about measurements? For this we will need to invoke a new mathematical beast called Operators

1. An operator is a quantity that "operates" on any element of a vector space and yields another element of the vector space:
$$\mathcal{O}|\eta\rangle = |\chi\rangle \tag{2.8.5}$$
Where $|\eta\rangle$ and $|\chi\rangle$ are *ket* vectors belonging to some n-dimensional vector space.

2. For simplicity we could look at rotation operators in 3-dimensions. For example, consider the unit vector $\hat{\imath}$ in 3-dimensions. A rotation operator about the z-axis converts $\hat{\imath} \rightarrow \hat{\jmath}$, the unit vector along the y-direction. Such a rotation operator conforms to the definition in Eq. (2.8.5) and is hence an operator in this sense. But this definition also applies to any general transformation in three-dimensions that takes an arbitrary vector $\vec{r}$ to $\vec{r'}$.

3. Every experimental measurement has a mathemaically corresponding operator!! Operators and vectors spaces (which we have already discussed using the Dirac notation) form a basic tool in quantum mechanics.

4. We will now introduce a specific kind of an operator. This operator is called the momentum operator and has the following form:
$$\hat{p} = -\imath\hbar\frac{\partial}{\partial x} \tag{2.8.6}$$
Note that we have seen $\hbar$ before in Eq. (2.2.9) and the section of wave-particle duality. The full theoretical reason for the choice of the momentum operator in Eq. (2.8.6) is based on the analogy to generator functions for infinitesimal translation in classical mechanics. This is nicely discussed in Section 1.6 (on page 44) of Sakurai. I urge you to read it.

5. We will see that every observable quantity has an operator associated with it in quantum mechanics and momentum is an observable quantity.

6. We noted above that an operator is one that acts on a vector and converts it to a different vector. Is it possible that an operator can act on some vector and not change it? That is,
$$\mathcal{O}|\eta\rangle = \imath|\eta\rangle \tag{2.8.7}$$

where $\wr$ is a number. Is this possible? Indeed, as we will see, for every operator that we will see in this course, there will always exist "special" *ket* vectors that do not change (only get re-scaled) on the action of some operator. These "special" *ket* vectors are called *eigen-vectors* of the operator $\mathcal{O}$. Every operator has a set of *eigen-vectors*. (Yes, a set of them.) The "special" numbers $\wr$ are called the *eigenvalues*. The term *eigen* comes from German; it means *characteristic*. So we are trying to say that the set of *eigen-vectors* and *eigenvalues* are characteristic of the operator they are obtained from. We will see more on this later as we solve quantum problems.

7. Since every operator has an eigenvector, what is the eigenvector for the momentum operator in Eq. (2.8.6)? To answer this question, lets try the action of the momentum operator in $\exp\{\imath kx\}$:
$$-\imath\hbar\frac{\partial}{\partial x}\exp\{\imath kx\} = \hbar k\exp\{\imath kx\} \tag{2.8.8}$$
You can check that this is true by differentiating the left hand-side once with respect to x. It is left as **homework** for the student to prove Eq. (2.8.8). The eigenstates of the momentum operator may also be represented by the *ket* $|k\rangle$. (Note: $k = \frac{2\pi}{\lambda}$.)

2.8.1 The coordinate and momentum representation and the Wavefunction

1. We shall also note here that the set $\{|n\rangle\}$ represented in Eq. (2.7.3) is a discrete set. How do we know this is discrete, the summation in Eq. (2.7.3) has a countable number of terms. In three-dimensional the summation in Eq. (2.7.3) has three terms; in four-dimensions it has four terms and in n-dimensions the summation in Eq. (2.7.3) has n terms. In the next section we will discuss a continuous representation which is basically obtained by converting the summation in Eq. (2.7.3) into an integral:
$$\sum \rightarrow \int \tag{2.8.9}$$
At this point it will be useful to review some of your calculus. In particular we would like to remember that the integration is "the limit of a sum". Hence the integration is very similar to a sum, but only has infinitely many terms in it. Hence the correspondence in Eq. (2.8.9) makes sense.

2. The eigenstates of momentum for a *continuous* representation which we discussed earlier (Eq. (2.8.9).
$$\int dk\,|k\rangle\langle k| = 1 \tag{2.8.10}$$
Why continuous? The k in Eq. (2.8.8) can take on any real value and $\exp\{\imath kx\}$ would still remain an eigenstate of the momentum operator.

3. Eigenstates of many different kinds of "special" operators in quantum mechanics always form a complete set. We will prove this general statement in detail later in this class.

 ©2014, Srinivasan S. Iyengar (instructor)

4. Like the momentum operator, there is another kind of operator in quantum mechanics called the position operator.

$$\hat{x} |x\rangle = x |x\rangle \tag{2.8.11}$$

The eigenstates of the position operator form another important complete set of *ket* vectors that form a continuous representation.

$$\int dx |x\rangle \langle x| = 1 \tag{2.8.12}$$

5. As the name suggests, the variable "x" above is the position (in 3-dimensions or in n-dimensions, but it is easier to picture this in 3D). What this means all point in a 3-dimensional space (for example) form a complete set of *ket* vectors. (This point is *extremely* subtle.)

6. **The Wavefunction:** In the Stern-Gerlach experiments we represented the states using the *ket* $|SG_x\rangle$. More generally, the state of any system can be represented by a *ket*, say $|\psi\rangle$. Consider the inner product of the *bra* state $\langle x|$ with a *ket* vector $|\psi\rangle$, *i.e.* $\langle x | \psi\rangle \equiv \psi(x)$. This quantity is called the wavefunction. Hence the wavefunction is the inner product of the abstract *ket* vector that represents the state of the system (for example the state of the Stern-Gerlach experiment) with the position representation. We will discuss a lot more in the next few lectures regarding this "wavefunction".

7. In fact the story of quantum mechanics, as we are going to learn it, is the story of how to find the wavefunction of the system. Why is this important?

   (a) We noted that the wavefunction is obtained by the inner product of the abstract *ket* vector that represents the state of the system with the position representation. (This process of performing this inner product is also called a *projection*. Hence, the wavefunction is the projection of the abstract *ket* vector $|\psi\rangle$ on to the position representation.)

   (b) Since $|\psi\rangle$ represents the state of the system, (as the states in the Stern-Gerlach experiment fully represent the state of the system, in a similar fashion $|\psi\rangle$ contains all information about the system). we would like to know everything there is to know about $|\psi\rangle$.

   (c) What is the equation that gives us $|\psi\rangle$? It is called the Schrödinger Equation, which we will see soon.

   (d) **Properties of the Wavefunction:** We will simply state the required properties here. Later when we solve our first quantum mechanical problem (the particle in a box) we will see how these properties become necessary.

   - The Wavefunction must be continuous.
   - The wavefunction must have finite values in all space.
   - The wavefunction must be normalized. That is the integral of the square of the wavefunction over all space must be 1:

$$\langle \psi | \psi\rangle = \langle \psi| \left\{ \int dx \, | x \rangle \langle x | \right\} |\psi\rangle = \int dx \psi^*(x)\psi(x) = 1 \tag{2.8.13}$$

This condition is extremely important, mathematically. It allows only a certain kind of function to be a wavefunction: ones that are *square integrable*. It also implies that the length of the ket $|\psi\rangle$ is always 1.

- And finally the quantity $dx\psi^*(x)\psi(x) \equiv dx|\psi(x)|^2$ is interpreted as the probability density of the system. That is the probability of finding the system in a infinitesimal area of size dx around the point x.

 ©2014, Srinivasan S. Iyengar (instructor)

3 Summary of Dirac's notation:

	Normal 3D space	Hilbert Space
Vectors	$\vec{i}$	$\|\psi\rangle$
Dual Space	$\vec{i}^\dagger$	$\langle\psi\|$
Vector representations	$\vec{r} = a\hat{i} + b\hat{j} + c\hat{k}$	$\|\psi\rangle = \{\sum_{l=1}^{n} \|l\rangle \langle l\|\} \|\psi\rangle$ OR $\int dx \|x\rangle \langle x \mid \psi\rangle$
	$\vec{r} \equiv \begin{pmatrix} a \\ b \\ c \end{pmatrix} \equiv \begin{pmatrix} \vec{i}^\dagger \vec{r} \\ \vec{j}^\dagger \vec{r} \\ \vec{k}^\dagger \vec{r} \end{pmatrix}$	$\|\psi\rangle \equiv \begin{pmatrix} \vdots \\ \langle x_1 \mid \psi\rangle \\ \langle x_2 \mid \psi\rangle \\ \langle x_3 \mid \psi\rangle \\ \vdots \end{pmatrix}$
Matrix representations	$A \equiv \sum_{i=1}^{3} \sum_{j=1}^{3} A_{i,j} \vec{i} \vec{j}^\dagger$	$A \equiv \sum_{i,j} \|i\rangle \langle j\| A_{i,j}$
	$= \begin{pmatrix} A_{1,1} & A_{1,2} & A_{1,3} \\ A_{2,1} & A_{2,2} & A_{2,3} \\ A_{3,1} & A_{3,2} & A_{3,3} \end{pmatrix}$	A matrix with matrix element $A_{i,j}$
	$= \begin{pmatrix} \vec{i}^\dagger A \vec{i} & \vec{i}^\dagger A \vec{j} & \vec{i}^\dagger A \vec{k} \\ \vec{j}^\dagger A \vec{i} & \vec{j}^\dagger A \vec{j} & \vec{j}^\dagger A \vec{k} \\ \vec{k}^\dagger A \vec{i} & \vec{k}^\dagger A \vec{j} & \vec{k}^\dagger A \vec{k} \end{pmatrix}$	$A_{i,j} = \langle i\| A \|j\rangle$

 ©2014, Srinivasan S. Iyengar (instructor)

	Normal 3D space	Hilbert Space
Vectors	$\vec{i}$	$\|\psi\rangle$
Orthonormality of the vector space	$\vec{i}^{\dagger}\vec{j} = \delta_{i,j}$	$\langle i \|j\rangle = \delta_{i,j}$
		$\langle x \|x'\rangle = \delta(x - x')$

 ©2014, Srinivasan S. Iyengar (instructor)